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THE APPLICATION OF KRIGING TECHNIQUE TO MATHEMATICAL MODELLING OF ESTUARINE WATER QUALITY

by
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B.Sc

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Abstract

It is essential that estuarine modelling and surveying are carried out simultaneously because not only does the latter provide data required by the former but also the former is verified with data from the latter. This study integrates both research subjects from the panoramic point of view, aiming at improving modelling accuracy and reliability and increasing survey efficiency.

Partially stratified estuaries are the most difficult types of estuaries to be modelled, in particular, the velocity field in such an estuary. A review of two commonly used methods to determine the velocity field, i.e., theoretical method and empirical method, revealed their inadequacies in real applications. Thus, a new approach using Kriging technique was originated and was tested on a finite element model of water quality. The model was formulated using a Galerkin-finite element method and was programmed in Fortran. Comparison between the simulation results and the field measurements for a salinity intrusion showed a high simulation accuracy. It is believed that the model in combination with the new approach would be a useful tool for estuarine modelling.

The generalized Kriging method ensured that the new approach would be appropriate in practice. It was also applied to the investigation of sampling stations in the partially mixed estuary of the River Tees. It is essential to know how many sampling stations should be used and how they should be positioned. Two procedures were designed for solving the survey problems. They were the procedure of overall variance and the procedure of re-estimation. These procedures were capable of quantifing the relative significance of each sampling station and detecting redundant sampling stations. The 1975 survey was investigated, and useful conclusions were obtained.

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Chapter 1 Introduction

A healthy environment is vital to the existence of all kinds of creatures living on the earth. Without it, the detrimental consequences to mankind are enormous. The environment has been under threat due to the disregard of human activities. Firstly, pollution caused by pollutants in forms of waste gases, waste solids and waste liquids from industries and communities has caused deterioration in air quality and water quality in surface water bodies like rivers, lakes, estuaries and coastal waters and in subsurface water bodies like acquifers as well. A vivid recent example of water pollution is the incident of seal deaths caused by polluted coastal waters in Europe. Secondly, destruction of ecological balance has been affecting and worsening the whole environmental system. A typical example is the deforestation and burning down of forests in Africa and South America, causing changes to global green house effect. Therefore, environmental protection is important for the future of mankind.

Fortunately, people are becoming more and more concerned about the safety of their environment. Pollution control has been the first problem to be tackled. There are two ways to control pollution. First, pollutant discharges are strictly prohibited. Second, a controlled amount of pollutant discharges may be allowed under the condition of causing no severe pollution by certain standards. The first way is ideal because there is absolutely no pollution caused, but is not realistic because it requires all wastes to be treated completely before discharging. In comparison, the second way is scientific and economical because it considers the ability of the environmental medium either water or air to dilute and purify a reasonable amount of wastes and requires proper control of waste discharges. Hence, the crux of the pollution control problem is how to quantify the proper waste discharges without violating a set environmental standard.

Control of water pollution has always been at the forefront of pollution research. Estuaries have become some of the most polluted stretches of water because historically it was assumed that they had an infinite capacity for self purification. The last few decades have shown this assumption to be erroneous. A rational method of estuarine pollution control is to use models to predict changes of water quality under various waste loads, thus rational decisions on reduction of discharges may be drawn from modelling studies. At present, there are many types of estuarine models, but the most popular types are mathematical models which are based on the solutions of the equations of motion and mass transport. These mathematical models have a strong theoretical basis. Theoretically, they are able to simulate all the complicated processes involved as ever increasing computing power and robust numerical methods are made available. However, those complicated processes are represented in models by model parameters such as coefficients of diffusion and dispersion representing mixing processes, drag coefficient representing bed stress variation etc.. The determination of model parameters is the most difficult part of modelling work because these parameters can not be expressed as known functions and need extensive field data to determine them.

Among estuarine models, models of partially mixed estuaries are the most difficult type to deal with. This type of model was developed later than the models for other types of estuaries mainly due to the difficulty in solving the coupled equations of motion and mass transport. Such a difficulty no longer poses an obstacle as more robust solution techniques have been developed. After the early 70's, a number of mathematical models were developed for partially stratified estuaries. Generally, a water quality model consists of a hydrodynamic submodel and mass transport submodel and a biochemical submodel. The hydrodynamic submodel provides velocity data required by the mass transport submodel. As convection is a dominant part of mass transport in partially stratified estuaries, the hydrodynamic model plays an important role in producing satisfactory results for the mass transport submodel. The determination of model parameters is more difficult to establish for hydrodynamic models than for mass transport models. There have been many studies on parameters used in mass trasport models but relatively there is insufficient research on parameters used in hydrodynamic models. Thus, before operational hydrodynamic models may be used, there must be sufficient research to quantify the hydrodynamic parameters properly. However, the use of hydrodynamic models is not the only approach to derive velocity fields for mass transport models. Another common approach uses field velocity data to fit empirical functions as input of velocity fields. This approach has limitations in accuracy and may be inconvenient in use. Therefore, there is a need to use a more practical approach to prepare velocity fields for mass transport models. To develop such a practical approach become part of the study in this thesis. Estuarine modelling cannot be implemented without estuarine surveying to provide essential data, and sufficient data can not be collected without using sufficient sampling stations. The term "sufficient "is so vague that it ought to be quantified. The assessment of estuarine surveys became another part of the study in this thesis.

The work presented in this thesis is arranged as follows. The research begins with a literature review showing the status of estuarine modelling, previous research on the River Tees, and motives of this work in chapter 2. Following are the description of the Kriging technique and its application to the River Tees surveying in chapter 3 and chapter 4. Chapter 5 introduces numerical methods. In chapter 6, the water quality model is formulated using Galerkin-finite element method. Chapter 7 presents the Kriging-finite element model of water quality with its application. In chapter 8, conclusions are drawn from the work and recommendations are made for further research.

Chapter 2 Literature Review

2.1 Introduction

Estuaries are meeting places of salt water and fresh water and are governed by tidal action seaward and by river flow landward. According to their salinity structure, estuaries can be classified into three major hydrodynamic types: highly stratified, partially mixed and well mixed(see Fig.2.1). In highly stratified estuaries, fresh water moves seaward on top of the salt water and there exists a sharp interface between the fresh water and salt water. In contrast, in well mixed estuaries, fresh water is vertically mixed with salt water. Partially mixed estuaries lie between the two extreme types because they have a significant vertical salinity gradient.

Estuaries have been extremely important in the world's development because of their large amount of water, sheltered anchorages and the navigational access to hinterlands. Therefore, they are the places where industries and population are always increasing. As a result, increasing amounts of wastes from industrial and domestic effluents are produced, and are dumped into estuaries. The effects of the wastes on estuarine water quality must be known or predicted if the water quality is to be maintained to a certain standard. For example, no nuisance standard is set as dissolved oxygen $\nless 1mgl^{-1}$ and no surface slick of oil and a limit on suspended solids(Elliott and James, 1985). To investigate the pollution problem, the only effective method is to use an estuarine model.

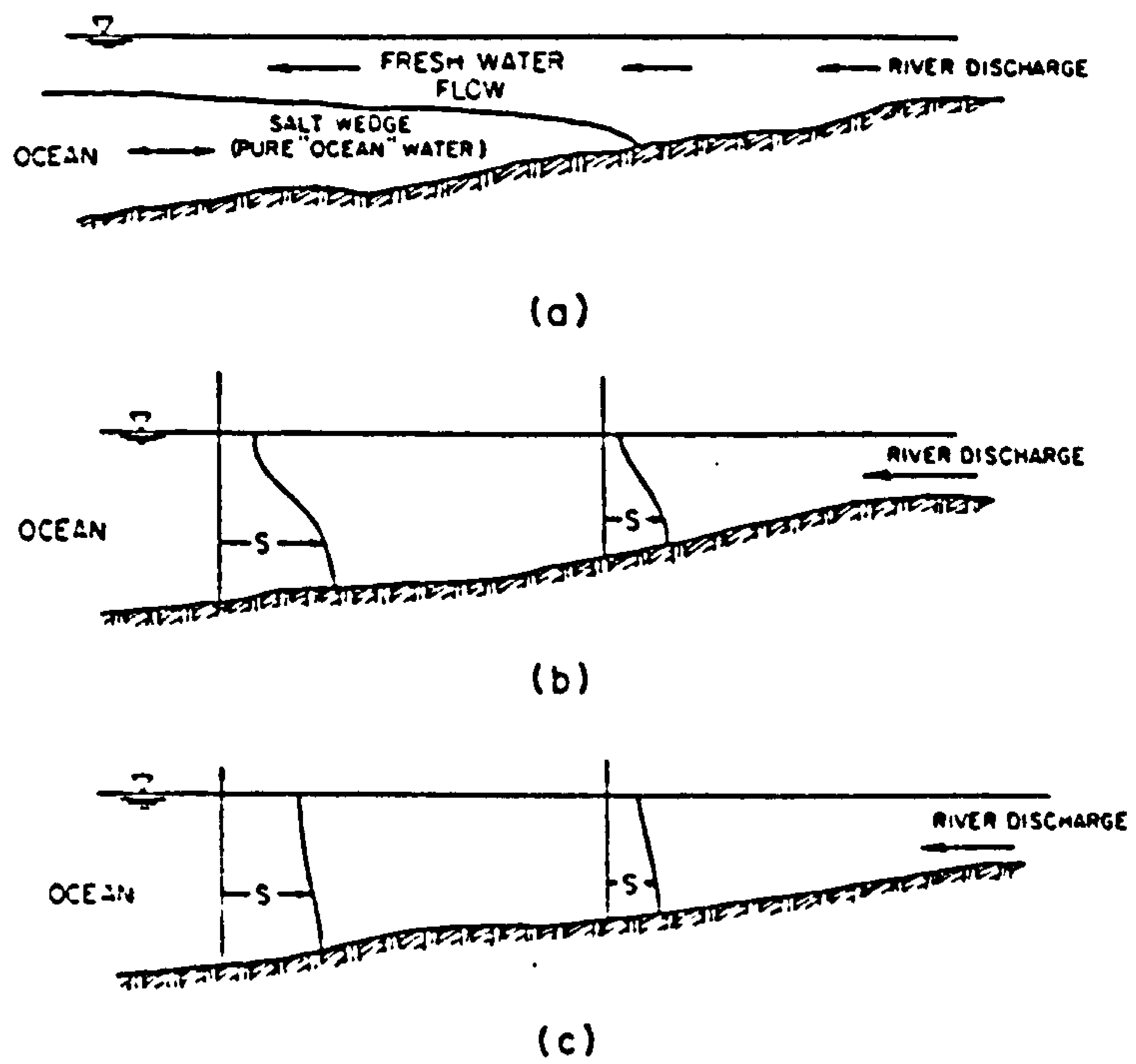

Fig 2.1 Salinity distribution along the axes of

(a) a highly stratified estuary

(b) a partially mixed estuary

(c) a well mixed estuary

(After, Fisher etc, 1979)

2.2 Estuarine Modelling

The objective of estuarine modelling is to reproduce the major features of estuarine circulation in order that prediction can be made of overall water quality in various cases of pollutant discharges. Among various models, each of them can be assigned to one of the four types: analytical models, simulation models, hydraulic models and numerical models. The main features of each type of model will be reviewed next with an emphasis on numerical models.

Analytical Models

The majority of analytical models are based on direct solutions to diffusion-advection equations(Harleman, 1966; O'connor, 1965; Holley and Harleman, 1965). These equations are usually greatly simplified so that an analytical solution may be derived. The simplification may be done by reducing the number of dimensions, assuming constants for all model parameters and regulating boundary conditions. The most common type of analytical models are one dimensional and have been used in the solution of general problems in the homogeneous tidal zone. As analytical models are idealized forms of physical situations, their application is limited.

Simulation Models

Simulation models are based on the concept of single mixing operation(Ketchum, 1950) and attempt a direct simulation of the bulk physical processes involved. This type of model does not consider the actual mixing processes in estuaries and assumes that the estuary is divided longitudinally into a number of segments. Each segment is assumed to be uniformly well mixed. Most simulation models have been applied to well mixed or slightly stratified estuaries(Preddy and Webber, 1963; Downing, 1963), however, a simulation model was also developed for a partially mixed estuary by Pritchard(1969). This type of model is limited to the steady state situation and is very difficult to extend into the time dimension.

Hydraulic Models

A hydraulic model is an attempt to reduce a prototype estuary to a small observable scale by the laws of scaling(Yalin, 1971; McDowell and O'connor, 1977; Harleman, 1971). Hydraulic models have the advantage that the natural topography can be reproduced in detail. Moreover, the tidal rise and fall at seaward and the river flow at landward can be made to vary continuously with time at will. Even wind and Coriolise Force can be included. The greatest single merit of hydraulic models is their capacity to reproduce the intricate three dimensional flow in a large estuary. Building a hydraulic model is expensive but using one that exists is relatively simple and cheap. Hydraulic models are able to produce reasonable answers to many estuarine problems. However, one should be reminded of the fact that a hydraulic model is not an exact replica of the prototype as nature itself is very complex and defies exact simulations. All hydraulic models are built in a form of distorted and reduced prototype so results from them should be treated cautiously.

Numerical Models

Numerical models are based on the computational solution of a set equations that are thought to describe the natural processes. The set of equations are the governing equations for hydrodynamics and the governing equations for solute conservation. These equations belong to the type of partial differential equations with initial and boundary conditions. They are the most complicated forms of differential equation, and no analytical solutions can be derived for such problems unless the problems are very idealized. Numerical methods are useful tools to solve differential equations for approximate solutions. Thus, numerical models use a particular numerical method to solve the set of governing equations of the problem. Mathematically, all existing estuarine numerical models may be categorized into two groups: finite difference models and finite element models, however, this is not an exclusive classification. Dimensionally, numerical models may be categorized into three groupes: one dimensional models, two dimensional models and three dimensional models. In terms of time scale, numerical models may be categorized into three groupes: steady state models, tidally averaged models and dynamic or time dependent models. Numerical models are described below with examples according to the dimensional treatment of the model.

One dimensional models are used for estuaries in which complete cross-sectional mixing may be assumed and the average concentration of a water parameter can be expressed as a function of distance along the length of the estuary (and or time). This type of model is relatively simple and easy to establish and solve mathematically, but it does not mean that those models are less important and useful. In principle, the simplest model that can solve the problem is the one to use. Examples of one dimensional finite difference models are those developed by Leendertse(1970,1971), Mollowney(1972), one dimensional finite element models are those by Dailey and Harleman(1973), Guymon(1970).

Two dimensional numerical models are used for estuaries in which either complete vertical mixing or lateral mixing be assumed. Thus, there are two types of two dimensional numerical models: vertically integrated and laterally integrated. Vertically integrated two dimensional models are often used in wide and shallow estuaries or bays. The majority of the existing two dimensional models belong to this type. Examples of vertically integrated two dimensional finite difference models are Falconer(1986), Apelt and Szewczyk(1973), and finite element models are Adey and Brebbia(1973), Guymon etc. (1970), Norton and King(1982). Laterally integrated two dimensional models were developed later than vertically integrated two dimensional models and only began to appear in publication after the early 70's. The main reason was lack of a more robust solution technique to solve the coupled equations of motion and salt transport simultaneously for representing gravitational circulation. This type of model is essential to study partially mixed estuaries which exhibit significant vertical and longitudinal variations in density and water quality conditions. The examples of laterally integrated finite difference models include Blumberg(1977), Hamilton(1974), and finite element models include Spaulding(1979), King etc (1973), Gee and MacAthur(1978), MacArther and Norton(1980).

Three dimensional models are used for estuaries which exhibt variations of water quality conditions along and across the estuary and with depth. Mathematically, this type of model fully represents all the three dimensions and does not include any simplifications in the mathematical description. However, like two dimensional models, even more data are required to specify three dimensional model parameters while they are the most expensive models to run computationally. These factors must be considered when selecting model type. Examples of three dimensional finite difference models are Leedertse and Liu(1973, 1975), Hess(1976), Capony(1976), Blumberg and Mellor(1978), Sheng and Butter(1982), and finite element model is King(1982).

Hybrid Models

Each type of model previously described has its advantages, disadvantages and limitations. Some of model formulations may be complementary to each other. For example, a hydraulic model may be used to supply boundary condition data for a numerical model or an analytical model may be used to check the accuracy of another type of model. Combinations among different types model could be various. A good example of such a hybrid model is Columbian river hybrid modelling system(McAnally etc. 1984) which combines hydrauic model, two dimensional numerical model, and analytical model in an integrated solution scheme.

Mixing Processes

The equations of motion and transport usually involve temporal and spatial averaging to make them tractable and practicable in time-smoothed two or one dimensional forms. As a result, new terms appear in the simplified equations. They are defined as turbulent viscosity, diffusivity and longitudinal dispersion coefficient. They are derived by analogy with Newton's Law of viscosity and Fick's First Law. These coefficients must be specified either theoretically or experimentally. The mixing processes are often very complicated so that there is still no predictive formula that works in general. It is necessary to properly represent mixing processes in estuarine models, particularly, in a one dimensional model where longitudinal dispersion plays a vital role in mass transport. A lot of research work has been directed to the representation of mixing processess. Different aspects of the research may be found in the work of those authors: Fish(1966, 67a, 67b, 68, 72), Fish etc.(1979), James and Park(1986), Park(1985), McCutcheor(1983), Delf(1979), Odd(1978), Christodoulou etc (1976), Beer(1983).

2.3 Previous Research on the River Tees

Major research on the River Tees began in the late 60's and centered around the problem of its water quality. Along with the research, many field surveys have been carried out to provide essential data. With the available data, mathematical models of water quality have been developed, and the mechanism of mixing processes have also been studied. In the following section, these aspects of research will be described briefly.

The first two dimensional model was developed by Hobbs and Fawcett(1972) for the investigation of water quality in the River Tees. At that time, the two authors were among the fewer pioneers to develope a time dependent model suitable for stratified estuaries. The model uses a finite difference method to solve the equation of mass transport. As was claimed by Hobbs(1970), it is impractical to collect sufficient field data to specify the velocity fields in the detail required by a mathematical model except in the very special circumstances of a laboratory tidal flume. An empirical velocity distribution was therefore used. By assuming that the hydrography and the fresh water flow are known, velocities were specified *a priori* from field data and the fluid continuity equation. No application was made to any particular water quality problems at the time the paper was published, and also no later description is available in the literature. Another two dimensional model was developed by Farraday(1973) as his Ph.D research. A Galerkin-finite element formulation was adopted in the model. It was proved that the finite element method is superior to the finite difference method for the solution of the differential equations of mass transport in estuaries. The field data recorded in the 1970 survey were resolved into a tidal and a periodic residual components by harmonic analysis. Then, empirical functions were fitted to each component to determine velocity field for the model. The model was shown to reproduce salinity data successfully. A one dimensional model was also developed to compare with the two dimensional model. The solution to a problem involving the continuous injection of a pollutant in the estuary showed that the one dimensional model is not suitable for solving the pollution problem in stratified estuaries.

A one dimensional finite difference model by Hobbs was used by Elliott et ae (1977) as the basis for an economic study of effluent discharges to the River Tees(Charles etc, 1977). The detailed descriptions of this model can be found in a separate unpublished report(Elliott, 1979). The longitudinal velocity is determined in the model from a knowledge of the estuary geometry, the tidal variations with respect to space and time, and fresh water inflow rate, using the principle of mass continuity. During the validation of the model using data from the 1970 survey, particular attention was centered on the performance of the 'effective longitudinal dispersion coefficients '. It was found that the value of the coefficient corresponded well with the experimental value. An objective assessment of the one dimensional model was provided in the study report.

A successful water quality model must represent its mixing processes correctly and a better understanding of the mixing processes is therefore indispensable. This important area of research has been pursued by Lewis(1979, 1981, 1983, 1987) using extensive data. Transverse velocity and salinity variations were observed at four cross-sections and their effect in salt flux was studied(Lewis, 1979). A further study using the 1975 Tees survey data showed the relative significance of each different mixing factor and highlighted the important components of the mixing processes(Lewis, 1981, 1983). A recent study(Lewis, 1987) on shear stress variations in the estuary provided further insight on the factors effecting drag coefficients and bed stress which may be used as boundary condition at the bed for the solution of the hydrodynamic equations. This work has made it possible to provide representative data for one of the most important parameters in hydrodynamic models.

All the research discussed above relies on comprehensive information of the estuary. Many surveys have been carried out on the River Tees. The first major survey was in 1935 under the direction of the Department of Scientific and Industrial Research. In 1966, preliminary surveys were made by the Water Pollution Research Laboratory(WPRL) at the request of Massers J. D. and D. M. Watson, Consulting Engineers. In 1969, a joint survey by ICI and Water Pollution Research Laboratory was carried out using seven stations for a period of nine days. In 1970 and 1975, two more comprehensive surveys were carried out by the joint forces of ICI, Teesside CBS, the WPRL and the NRA using nine and eight stations respectively in two seperate periods of five days covering neap and spring tides.

2.4 Motives of the Present Research

There already exist a two dimensional finite difference model and a two dimensional finite element model developed for the River Tees. It seems unnecessary to develop another similar model. But, before making a positive answer to such an issue, it is advisable to assess the two models from the point of their applicability.

The finite difference model has great difficulties in approximating irregular boundaries. Farraday(1973) found the finite element method is more suitable than the finite difference method for modelling the irregular, time dependent estuary geometry. Unfortunately, the programming language used in Farraday's model is Algol-60 which is no longer in widespread use. Existing computing facilities almost exclusively use Fortran and Pascal as their programming languages. Therefore, a finite element model written in Fortran language is more desirable.

Although the two models use different numerical methods, their approach to the determination of flow fields are very similar. They both make use of empirical velocity distributions by fitting field velocity data. This empirical approach is a process based on further assumptions which are difficult to prove. Therefore, it is doubtful whether the flow pattern used in the model represents the real flow pattern in which the field velocities were measured. A velocity field input to the model specified directly from field data has always been excluded because it is regarded impractical to collect sufficient field data specifing velocities at sufficient points required by a mathematical model. It is quite true in the sense that it is out of the question to measure velocity values at all the points required by a model. However, two questions are worth consideration

(1) Is it necessary to collect such detailed data?

(2) Is it possible to specify velocity field basing on limited amount of data by estimation?

Research on the two questions may lead to an alternative approach for incorporating flow fields data into water quality models.

Many field surveys have been carried out in the past years. Most of them used a number of sampling stations aiming at producing accurate distribution of the sampled parameters in the estuary. These surveys are usually guided by experienced personnel using their intuition or experience. As major estuarine surveys are costly to operate, even for later similar surveys, it would be useful to know how many sampling stations should have been used and where they should have been positioned. Such conclusions may be derived from analyses of data from previous surveys.

Chapter 3 Theory of the Kriging Technique

3.1 Introduction

There are many problems in engineering and science where the data collected in space (and/or in time) are usually not sufficient for a particular purpose, e.g., drawing contour maps of the measured variables or calculating averages of the measured variables over domains. To solve such problems, there are two approaches available. The first approach is to increase the number of data measurements directly so that the contour drawing or average value calculation can be satisfactorily performed. The second approach is to increase the number of data measurements indirectly so that the same objective can be achieved.

Most data collection programmes are financially expensive to operate. For example, measuring water parameters in estuaries involves both boats and manpower which are expensive to support.

The second indirect way depends on a mathematical method to derive more information from the limited data. This mathematical method is the estimation technique. There are various estimation methods available, such as the spline fit method and the least square method. The applicability of each each method varies with the property of measured variables. For example, the spline fit method can only be applied to those variables which change smoothly in space (and/or in time) so that polynomial functions can be fitted to the data points. Many variables involved in natural phenomena are so changeable that a deterministic mathematical description fails to represent them while a pure statistical description may not fit them either. Particularly, those normal estimation methods become suspect when the accuracy of estimations is assessed. In order to estimate those variables, a new method is needed which is neither deterministic nor based on frequency distributions.

Matheron(1971) described a regionalized variable as a variable which develops in space (and/or in time) and possesses a certain structure. A regionalized variable differs from an ordinary random variable which is defined as a variable taking a certain number of numerical values according to a certain probability distribution. Two realizations of a regionalized variable which differ in spatial location display generally a non-zero correlation. In many cases the closer the measurement points to each other, the closer the measured values. In contrast an ordinary random variable has successive realizations which are uncorrelated. The term "structure "is refered to this spatial correlation of regionalized variables. Regionalized variables can be classified into two categories: stationary and non-stationary. In the former the variable has no systematic trend in space, and in the latter the variable has a definite trend in space. Here, by a trend it means that the variable increases or decreases in certain directions.

From the concept of a random variable, a more powerful concept called random functions can be formed. A random function expressed as $Z(x, \xi)$ varies with both the spatial coordinate system x(X,Y,Z) and the state variable ξ in the ensemble of realizations. Thus, $Z(x, \xi_1)$ is a realization of $Z(x, \xi)$; $Z(x_0, \xi)$ is a random variable, i.e., the ensemble of the realizations of the random function $Z(x, \xi)$ at x_0; $Z(x_0, \xi_1)$ is the single value of $Z(x, \xi)$ at x_0 for realization ξ_1. The definition of random functions expresses the random and structured aspects of a regionalized variable. This concept lays the cornerstone for the estimation method to be introduced next.

On the basis of both the theory of regionalized variables and the theory of intrinsic random functions, Matheron(1971,1973) developed an estimation method named after D. G. Krige, who first applied some of the concepts underlying this method to estimate the average grade and total tonnage of the ore reserve of the South African Mines(Krige, 1978). According to the original definition given by Matheron, Kriging is the probabilistic process of obtaining the best linear unbiased estimator of an unknown variable, "best "being taken here in the sense of minimization of the resulting estimation variance. This method has been widely used in mining engineering, geology, hydrogeology, hydrology, and even in the petroleum industry(Guarascio, 1975; Joural, 1978; Verly, 1983; Marseley,1984; Delhomme, 1979; Bras, 1985). It has been proved to be a very effective estimation tool.

Suppose there are n points of measurements of a regionalized variable: $Z(x_1), Z(x_2), ..., Z(x_n)$, where ξ has been omitted for simpilicity, then an estimation at any point can be defined as a linear combination of n measured values:

$$Z^*(x) = \sum_{i=1}^{n} \lambda_i Z(x_i) \qquad 3.1$$

where λ_i is a weighting coefficient to point x_i. It is the method of determination of the weighting coefficients that distinguishes various estimation methods. In the Kriging method, The n weights λ_i are calculated to ensure that the estimation is unbiased and the estimation variance is minimal. The two conditions are expressed as

$$E[Z^*(x) - Z(x)] = 0 \qquad 3.2$$

$$Var[Z^*(x) - Z(x)] = minimum \qquad 3.3$$

where Z(x) is a real value at point x. From the equations 3.1-3.3, it can be concluded that the Kriging method is a best linear unbiased estimator.

As a regionalized variable may be stationary or non-stationary, the Kriging method dealing with the two cases differs. The classification of all the Kriging methods is shown in Fig. 3.1. Following sections will describe each of them respectively.

3.2 Ordinary Kriging

Ordinary Kriging is used when the regionalized variable is stationary. Mathematically, whether a regionalized variable is stationary or non-stationary can be determined through the mathematical expectation of the random function $E[Z(x,\xi)]$. If $E[Z(x,\xi)] = m$(constant), then it is said to be stationary; otherwise, it is said to be non-stationary. In the stationary case, the Kriging method may be different under the second-order stationarity hypothesis and the intrinsic hypothesis.

A random function is said to be second-order stationary when:
(1) the mathematical expectation $E[Z(x,\xi)]$ exists and does not depend on the position x:

$$E[Z(x,\xi)] = m(x) = m \qquad 3.4$$

(2) for each pair of random variables $\{Z(x_i,\xi), Z(x_i+h,\xi)\}$, the covariance

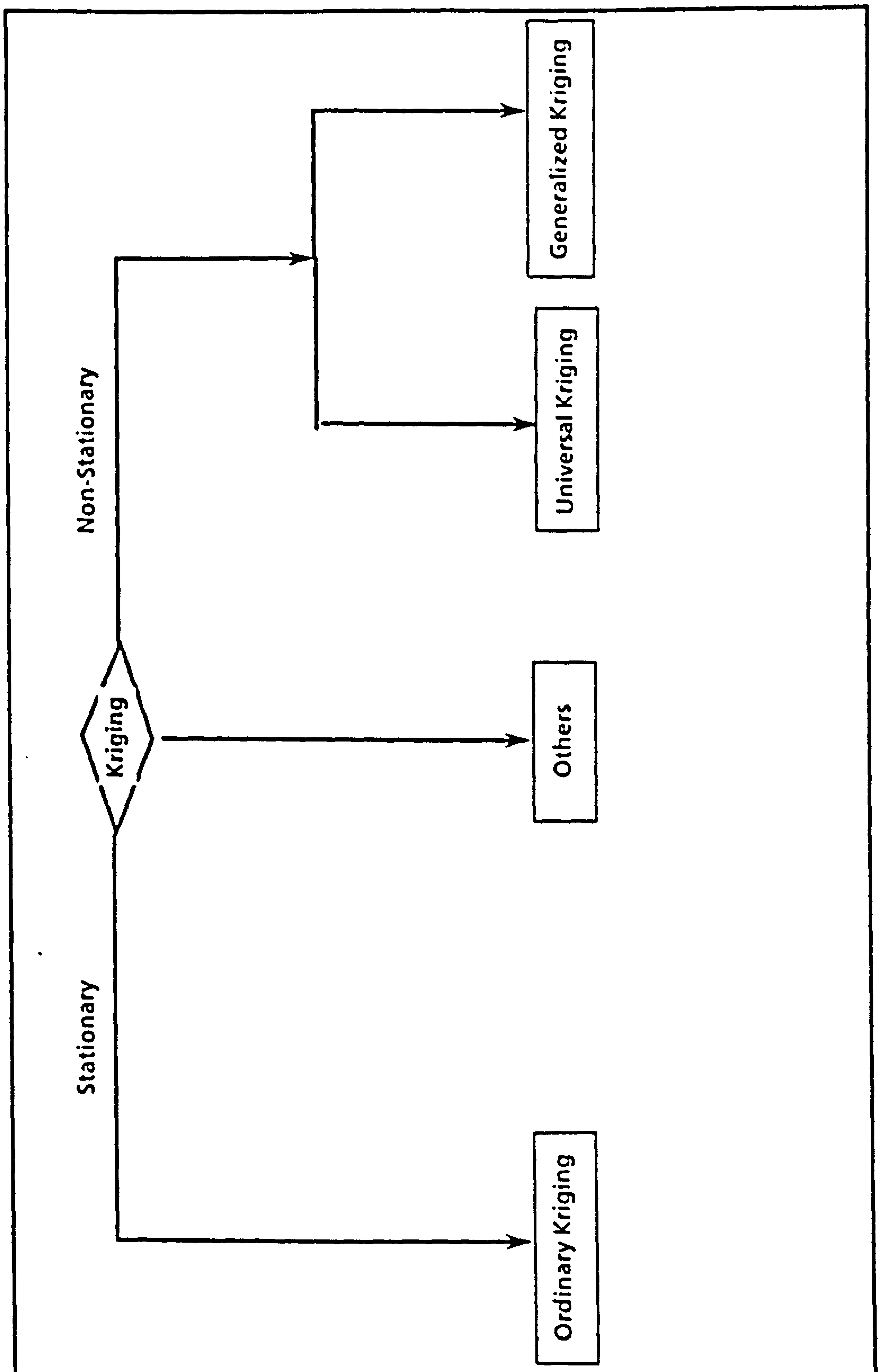

Fig. 3.1 The classification of the Kriging technique

exists and depends on the distance and not on the points of reference:

$$Cov[Z(x_i, x_i + h)] = E\{[Z(x_i, \xi) - m][Z(x_i + h, \xi) - m]\}$$
$$= C(h) \qquad 3.5$$

The hypothesis of second-order stationarity assumes the existence of a covariance. This covariance is the structure mentioned in the definition of a regionalized variable. Next, the "Kriging system "under the hypothesis of second-order stationarity is presented. As the constant m in equation 3.4 is generally unknown, it is treated as an unknown constant in the following derivation.

The estimator defined in equation 3.1 is a linear combination of the n data values. The n weights λ_i are calculated to ensure the satisfaction of the equations 3.2 and 3.3

Non-bias condition

Equation 3.2 is written

$$E[Z^*(x)] = E[Z(x)]$$

then, by equation 3.1 it can be written as

$$E[\sum_{i=1}^{n} \lambda_i Z(x_i)] = E[Z(x)]$$

As the summation sign can be exchanged with the mathematical expectation sign, the above equation is then written as

$$\sum_{i=1}^{n} \lambda_i E[Z(x_i)] = E[Z(x)]$$

By equation 3.4, the above equation becomes

$$\sum_{i=1}^{n} \lambda_i m = m$$

$$\sum_{i=1}^{n} \lambda_i = 1$$

Minimum estimation variance

The left hand side of equation 3.3 can be written as

$$Var[Z^*(x) - Z(x)] = E[(Z^*(x) - Z(x))^2] - E^2[Z^*(x) - Z(x)]$$

Because of the non-bias condition, the above equation become

$$Var[Z^*(x) - Z(x)] = E[(Z^*(x) - Z(x))^2]$$

The right hand side of the above equation can be further developed as follows

$$\begin{aligned}
E[(Z^*(x) - Z(x))^2] &= E[(\sum_{i=1}^{n} \lambda_i Z(x_i) - Z(x))^2] \\
&= E[(\sum_{i=1}^{n} \lambda_i Z(x_i))^2 - 2(\sum_{i=1}^{n} \lambda_i Z(x_i))Z(x) + Z^2(x)] \\
&= E[(\sum_{i=1}^{n} \lambda_i Z(x_i))(\sum_{j=1}^{n} \lambda_j Z(x_j)) - 2\sum_{i=1}^{n} \lambda_i Z(x_i)Z(x) \\
&\quad + Z^2(x)] \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i \lambda_j E[Z(x_i)Z(x_j)] - 2\sum_{i=1}^{n} \lambda_i E[Z(x_i)Z(x)] \\
&\quad + E[Z^2(x)]
\end{aligned}$$

From equation 3.5

$$E[Z(x_i)Z(x_j)] = C(x_i, x_j) + m^2$$

$$E[Z(x_i)Z(x)] = C(x_i, x) + m^2$$

Thus

$$E[(Z^*(x)-Z(x))^2]=\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j C(x_i,x_j)-2\sum\lambda_i C(x_i,x)+E[Z^2(x)]-m^2$$
$$=\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j C(x_i,x_j)-2\sum\lambda_i C(x_i,x)+C(0) \qquad 3.6$$

As can be seen from the above expression, the estimation variance has been expressed as a quadratic form in λ_i, λ_j. Now it can be minimized subject to the non-bias condition

$$\sum_{i=1}^{n}\lambda_i=1$$

The optimal weights are obtained from standard Lagrangian techniques by setting each of the n partial derivatives

$$\frac{\partial}{\partial\lambda_i}\{E[(Z^*(x)-Z(x))^2]-2\mu\sum_{i=1}^{n}\lambda i\}$$

to zero. This procedure provides a set of $(n+1)$ equations for $(n+1)$ unknowns. Thus, the "Kriging system "is

$$\sum_{j=1}^{n}\lambda_j C(x_i,x_j)-\mu=C(x_i,x) \qquad i=1,2,...,n$$

$$\sum_{j=1}^{n}\lambda_i=1 \qquad 3.7$$

Its matrix form is written as

$$\begin{bmatrix} C_{11} & C_{12} & \dots & C_{1n} & 1\\ C_{21} & C_{22} & \dots & C_{2n} & 1\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ C_{n1} & C_{n2} & \dots & C_{nn} & 1\\ 1 & 1 & \dots & 1 & 0 \end{bmatrix}\times\begin{bmatrix}\lambda_1\\ \lambda_2\\ \vdots\\ \lambda_n\\ -\mu\end{bmatrix}=\begin{bmatrix}C_{10}\\ C_{20}\\ \vdots\\ C_{n0}\\ 1\end{bmatrix}$$

where $C_{ij} = C(x_i, x_j), C_{i0} = C(x_i, x)$

The minimum estimation variance can be derived from equations 3.6 and 3.7 as

$$\begin{aligned} Var[Z^*(x) - Z(x)] &= E[(Z^*(x) - Z(x))^2] \\ &= C(0) + \mu - \sum_{i=1}^{n} \lambda_i C(x_i, x) \end{aligned}$$

When the constant m is known, the "Kriging system "is almost same, but the residual $Y_i = Z_i - m$ is used in stead of Z_i.

A full second-order stationarity assumption is very restrictive in practical problems where the mean value m is always unknown, and may not be constant so that the covariance and variance can not be computed directly, or where the variance C(0) is infinite. Therefore, a less stringent hypothesis than the hypothesis of the second-order stationarity is required to make the estimation possible. The intrinsic hypothesis only assumes
(1) the mathematical expectation exists and does not depend on the support point x

$$E[Z(x,\xi)] = m = constant$$

(2) for all vector h, the increment $[Z(x+h,\xi) - Z(x,\xi)]$ has a finite variance which does not depend on x

$$\begin{aligned} Var[Z(x+h,\xi) - Z(x,\xi)] &= E\{[Z(x+h,\xi) - Z(x,\xi)]^2\} \\ &= 2\gamma(h) \end{aligned} \qquad 3.8$$

where $\gamma(h)$ is called a semivariogram.

To compare the intrinsic hypothesis with the hypothesis of the second-order stationarity, it can be seen that the existence and stationarity of the semivariogram $\gamma(h)$ requires a weaker condition than the covariance C(h). This can be shown in the relationship between the second-order stationarity hypothesis and the intrinsic hypothesis as the former implies the the latter but the converse is not true.

The "Kriging system "under the intrinsic hypothesis can be derived in the same way as under the hypothesis of the second-order stationarity, but it is still worth indicating differences in the process of derivation.

Non-bias condition

$$E[Z^*(x)] = E[Z(x)]$$

leads to

$$\sum_{i=1}^{n} \lambda_i = 1$$

Minimum estimation variance

$$\begin{aligned} Var[Z^*(x) - Z(x)] &= E[(Z^*(x) - Z(x))^2] \\ &= E[(\sum_{i=1}^{n} \lambda_i Z(x_i) - (\sum_{i=1}^{n})Z(x))^2] \\ &= E[(\sum_{i=1}^{n} \lambda_i (Z(x_i) - Z(x))^2] \\ &= E[\sum_{i=1}^{n} \lambda_i (Z(x_i) - Z(x)) \sum_{j=1}^{n} \lambda_j (Z(x_j) - Z(x)] \\ &= E[\sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j (Z(x_i 0 - Z(x))(Z(x_j) - Z(x))] \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j E[(Z(x_i) - Z(x))((Z(x_j) - Z(x))] \end{aligned}$$

From equation 3.8, the semivariogram $\gamma(h)$ can be developed as

$$\begin{aligned}
\gamma(x_i - x_j) &= \frac{1}{2}E[(Z(x_i) - Z(x_j))^2] \\
&= \frac{1}{2}E[((Z(x_i) - Z(x)) - (Z(x_j) - Z(x)))] \\
&= \frac{1}{2}E[(Z(x_i) - Z(x))^2] + \frac{1}{2}E[(Z(x_j) - Z(x))^2] \\
&\quad - E[(Z(x_i) - Z(x))(Z(x_j) - Z(x))] \\
&= \gamma(x_i - x) + \gamma(x_j - x) - E[((Z(x_i) - Z(x))(Z(x_j) - Z(x))]
\end{aligned}$$

Thus,

$$E[((Z(x_i) - Z(x))(Z(x_j) - Z(x))] = \gamma(x_i - x) + \gamma(x_j - x) - \gamma(x_i - x_j)$$

Substituting the above relation into the previous expression

$$\begin{aligned}
E[(Z^*(x) - Z(x))^2] &= -\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j\gamma(x_i - x_j) + \sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j\gamma(x_i - x) \\
&\quad + \sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j\gamma(x_j - x) \\
&= -\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j\gamma(x_i - x_j) + 2\sum_{i=1}^{n}\lambda_i\gamma(x_i - x)
\end{aligned}$$

setting

$$\frac{\partial}{\partial\lambda_i}\{E[(Z^*(x) - Z(x))^2] - 2\mu\sum_{i=1}^{n}\lambda_i\} = 0$$

The "Kriging system "is

$$\begin{aligned}
&\sum_{j=1}^{n}\lambda_j\gamma(x_i, x_j) + \mu = \gamma(x_i, x) \qquad i = 1, 2, ..., n \\
&\sum_{j=1}^{n}\lambda_i = 1
\end{aligned} \tag{3.9}$$

Its matrix form

$$\begin{bmatrix} \gamma_{11} & \gamma_{12} & \cdots & \gamma_{1n} & 1 \\ \gamma_{21} & \gamma_{22} & \cdots & \gamma_{2n} & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \gamma_{n1} & \gamma_{n2} & \cdots & \gamma_{nn} & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{bmatrix} \times \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \\ \mu \end{bmatrix} = \begin{bmatrix} \gamma_{10} \\ \gamma_{20} \\ \vdots \\ \gamma_{n0} \\ 1 \end{bmatrix}$$

where $\gamma_{ij} = \gamma(x_i, x_j), \gamma_{i0} = \gamma(x_i, x)$

The minimum estimation variance is

$$\begin{aligned} Var[Z^*(x) - Z(x)] &= E[(Z^*(x) - Z(x))^2] \\ &= \sum_{i=1}^{n} \lambda_i \gamma(x_i, x) + \mu \end{aligned}$$

Comparing the "Kriging system "(3.7) and (3.9), it is found that the "Kriging system "(3.9) can be derived directly from (3.7) if $C(x_i - x_j)$ is replaced by $[-\gamma(x_i - x_j)]$.

The "Kriging system "has been derived under the intrinsic hypothesis, but little has been said about the semivariogram. A semivariogram represents the structure of a regionalized variable. It is important to find the correct semivariogram for accurate estimations. There are two ways to obtain a semivariogram. The first way is to use the definition given by equation 3.8, which can be expressed in a practical form as

$$\gamma(h) = \frac{1}{2n(h)} \sum_{i=1}^{n(h)} [Z(x_{i+h}) - Z(x_i)]^2$$

where n(h) is the number of pairs of data points whose distance is h. The semivariogram calculated directly from data tends to be rather lumpy, i.e., the noiser the data the less regular it appears to be . That is why the second way comes into use very often in practice. The second way fits model semivariograms which have been defined on theoretical or empirical grounds using available data. The principal types of model variograms employed in practice are:

(1) linear model

(2) h^λ model, $\lambda < 2$

(3) spherical model

(4) exponential model

(5) Gaussian model

These model functions and their curve forms are shown in Fig. 3.2

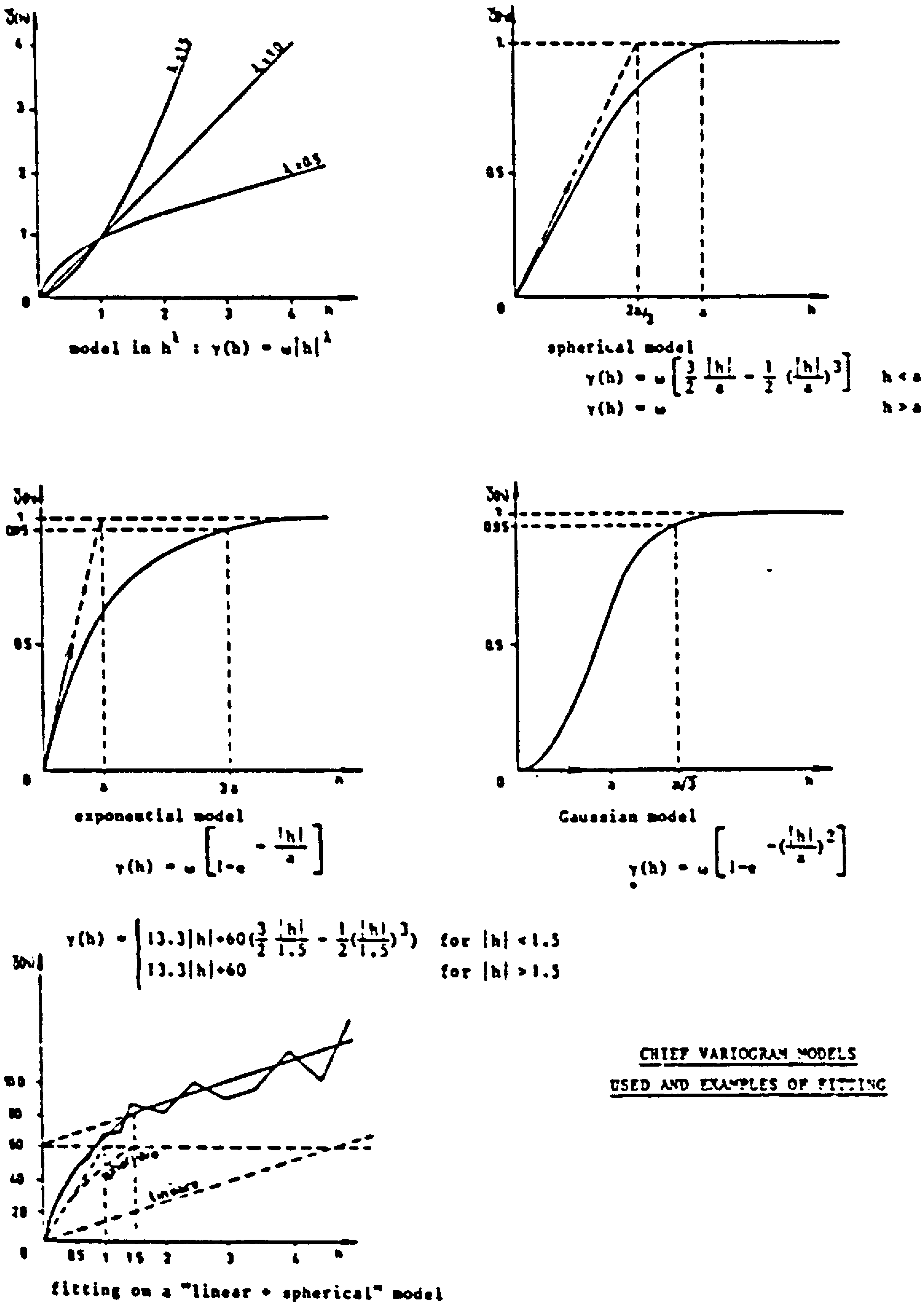

Fig. 3.2 Models of variograms

(After Marsily, 1984)

3.3 Universal Kriging

When the stationarity condition, i.e., $E[Z(x,\xi)] = m, constant$, is no longer satisfied, ordinary Kriging cannot be used. Universal Kriging was first used to the cases in which the mean constant can not be assumed. Since the focus of the present problem is an unknown m(x), universal Kriging proposes that the mean m(x) be regular and be modeled as a linear combination of ν basic functions $f^l(x)$ as

$$m(x) = \sum_{l=0}^{\nu} a_l f^l(x) \qquad 3.10$$

where the basic functions $f^l(x)$ are known functions, but the coefficients $a_l, l = 0, ..., \nu$ are unknown. Polynomial functions are commonly used for m(x) in particular. For instance, m(x) can be expressed in two dimensional coordinates(X,Y)

$$m(x) = a_0 + a_1X + a_2Y + a_3X^2 + a_4XY + a_5Y^2 + \dots$$

It should be pointed that universal Kriging is not universal either in theory or in practice. "universal "is used because the corresponding kriging estimation is unbiased whatever the unknown parameters a_l in equation 3.10. Although the form of the mean m(x) is known, it's value is still unknown because of its unknown coefficients a_l. Subsequently, the variogram $\gamma(h)$ cannot be calculated directly from data shown as

$$\begin{aligned}\gamma(h) &= \frac{1}{2}Var[Z(x+h) - Z(x)] \\ &= \frac{1}{2}E[(Z(x+h) - Z(x))^2] - \frac{1}{2}(m(x+h) - m(x))^2\end{aligned}$$

However, without a known form of semivariogram $\gamma(h)$, the Kriging system cannot be set up. The only way is to assume that the semivariogram $\gamma(h)$ is known. The "Kriging system "is derived for universal Kriging as follows

Non-bias condition

$$E[Z^*(x)] = E[Z(x)]$$

$$E[\sum_{i=1}^{n} \lambda_i Z(x_i)] = E[Z(x)]$$

$$\sum_{i=1}^{n} \lambda_i E[Z(x)] = E[Z(x)]$$

$$\sum_{i=1}^{n} \lambda_i m(x_i) = m(x)$$

Substituting equation 3.10 into the above equation, it becomes

$$\sum_{i=1}^{n} \lambda_i (\sum_{l=0}^{\nu} a_l f^l(x)) = \sum_{l=0}^{\nu} a_l f^l(x)$$

Interchanging the sum signs on the left hand equation, thus

$$\sum_{l=0}^{\nu} a_l (\sum_{i=1}^{n} \lambda_i f^l(x_i)) = \sum_{l=0}^{\nu} a_l f^l(x)$$

For any value of the unknown coefficients a_l the above equation exists only if

$$\sum_{i=1}^{n} \lambda_i f^l(x_i) = f^l(x) \qquad l = 0, 1, \ldots, \nu$$

Minimum estimation variance

$$Var[Z^*(x) - Z(x)] = E[(Z^*(x) - Z(x)]$$

Like the intrinsic case, it can be expressed as

$$\begin{aligned} Var[Z^*(x) - Z(x)] &= \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j E[(Z(x_i) - Z(x))(Z(x_j) - Z(x))] \\ &= -\sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j \gamma(x_i - x_j) + 2 \sum_{i=1}^{n} \lambda_i \gamma(x_i - x) \end{aligned}$$

Set

$$\frac{\partial}{\partial\lambda_i}\{E[(Z^*(x)-Z(x)]-2\sum_{l=0}^{\nu}\nu_l\sum_{i=1}^{n}\lambda_i f^l(x_i)\}=0$$

The "Kriging system "is written

$$\sum_{j=1}^{n}\lambda_j\gamma(x_i-x_j)+\sum_{l=0}^{\nu}\nu_l f^l(x_i)=\gamma(x_i-x) \qquad i=1,2,...,n$$

$$\sum_{i=1}^{n}\lambda_i f^l(x_i)=f^l(x) \qquad l=0,1,...,\nu$$

Its matrix form

$$\begin{bmatrix} \gamma_{11} & \gamma_{12} & \cdots & \gamma_{1n} & 1 & f^1(x_1) & \cdots & f^\nu(x_1) \\ \gamma_{21} & \gamma_{22} & \cdots & \gamma_{2n} & 1 & f^1(x_2) & \cdots & f^\nu(x_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \gamma_{n1} & \gamma_{n2} & \cdots & \gamma_{nn} & 1 & f^1(x_1) & \cdots & f^\nu(x_n) \\ 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ f^1(x_1) & f^1(x_2) & \cdots & f^1(x_n) & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ f^\nu(x_1) & f^\nu(x_2) & \cdots & f^\nu(x_n) & 0 & 0 & \cdots & 0 \end{bmatrix} \times \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \\ \mu_0 \\ \mu_1 \\ \vdots \\ \mu_\nu \end{bmatrix} = \begin{bmatrix} \gamma_{10} \\ \gamma_{20} \\ \vdots \\ \gamma_{n0} \\ 1 \\ f^1(x) \\ f^2(x) \\ \vdots \\ f^\nu(x) \end{bmatrix}$$

where $\gamma_{ij}=\gamma x_i-x_j, \gamma_{i0}=\gamma(x_i-x)$

Its estimation variation is

$$Var[Z^*(x)-Z(x)]=\sum_{i=1}^{n}\lambda_i\gamma(x_i-x)+\sum_{l=0}^{\nu}\mu_l f^l(x)$$

The prerequisite of using universal Kriging is that the semivariogram must be known beforehand. This is contradictory to the fact that $\gamma(h)$ can not be calculated directly from data. That is why universal Kriging is very limited in applications and a more general class of Kriging has been introduced.

3.4 Generalized Kriging

The generalized Kriging is based on the theory of intrinsic random function of order k (Matheron, 1973; Delfiner, 1976). The main advantage of this class of Kriging method lies in making the inference of the covariance possible in spite of the presence of a drift.

In the non-stationary case, the mathematical expectation of a random function $Z(x,\xi)$ is no longer constant

$$E[Z(x,\xi)] = m(x)$$

where m(x) is not known, but it may be assumed to be of a known form shown in equation 3.10 used in universal Kriging

$$m(x) = \sum_{l=0}^{\nu} a_l f^l(x)$$

the $f^l(x)$ are normally assumed to be basic monomial of a polynomial of order k, where $\nu = [\frac{(k+1)(k+2)}{2} - 1]$. In the two coordinate (X,Y) system, m(x) is expressed as

$$\begin{array}{lll} k=0 & m(x) = a_0 & \nu = 0 \\ k=1 & m(x) = a_0 + a_1X + a_2Y & \nu = 2 \\ k=2 & m(x) = a_0 + a_1X + a_2Y + a_3X^2 + a_4Y^2 + a_5XY & \nu = 5 \end{array}$$

As usual, an estimation at point x_0 expressed as

$$Z^*(x_0) = \sum_{i=1}^{n} \lambda_i Z(x_i)$$

Then, the error of the estimation is

$$\begin{aligned} Z^*(x_0) - Z(x_0) &= \sum_{i=1}^{n} \lambda_i Z(x_i) - Z(x_0) \\ &= \sum_{i=0}^{n} \lambda_i Z(x_i) \qquad (\lambda_0 = -1) \end{aligned}$$

The theory of the intrinsic random functions of order k proposes that if the weights λ_i of such a linear combination

$$\sum_{i=0}^{n} \lambda_i Z(x_i)$$

satisfy the following conditions

$$\sum_{i=0}^{n} \lambda_i f^l(x_i) = 0, \qquad l = 0, 1, \ldots, \nu \tag{3.11}$$

then

$$\sum_{i=0}^{n} \lambda_i Z(x_i)$$

may be called a generalized increment of order k because it filters out a polynomial of order k; and the variance of the generalized increment be expressed

$$Var[\sum_{i=0}^{n} \lambda_i Z(x_i)] = \sum_{i=0}^{n} \sum_{j=0}^{n} \lambda_i \lambda_j K(x_i - x_j) \tag{3.12}$$

where $K(x_i - x_j)$ is defined as a generalized covariance of the intrinsic random functions of order k.

Returning to the problem of deriving the "Kriging system ", the two criteria used before should be satisfied

Non-bias condition

$$E[Z^*(x_0)] = E[Z(x_0)]$$

It is expanded as

$$E[\sum_{i=1}^{n} \lambda_i Z(x_i)] = E[Z(x_0)]$$

$$\sum_{i=1}^{n} \lambda_i E[Z(x_i)] = E[Z(x_0)]$$

$$\sum_{i=1}^{n} \lambda_i m(x_i) = m(x_0)$$

Substituting equation 3.10 into the above equation, it becomes

$$\sum_{i=1}^{n} \lambda_i \sum_{l=0}^{\nu} a_l f^l(x_i) = \sum_{l=0}^{\nu} a_l f^l(x_0)$$

$$\sum_{l=0}^{\nu} a_l \sum_{i=1}^{n} \lambda_i f^l(x_i) = \sum_{l=0}^{\nu} a_l f^l(x_0)$$

$$\sum_{l=0}^{\nu} a_l \sum_{i=0}^{n} \lambda_i f^l(x_i) = 0 \quad (\lambda_0 = -1)$$

$$\sum_{i=0}^{n} \lambda_i f^l(x_i) = 0 \qquad l = 0, 1, \ldots, \nu \tag{3.13}$$

This condition is satisfied implicitly because the intrinsic random functions of order k satisfies equation 3.11, which can be written fully as

$k=0$	$\sum_{i=0}^{n}\lambda_i=0$		
$k=1$	$\sum_{i=0}^{n}\lambda_i=0$	$\sum_{i=0}^{n}\lambda_i X_i=0$	$\sum_{i=0}^{n}\lambda_i Y_i=0$
$k=2$	$\sum_{i=0}^{n}\lambda_i=0$	$\sum_{i=0}^{n}\lambda_i X_i=0$	$\sum_{i=0}^{n}\lambda_i Y_i=0$
	$\sum_{i=0}^{n}\lambda_i X_i^2=0$	$\sum_{i=0}^{n}\lambda_i Y_i^2=0$	$\sum_{i=0}^{n}\lambda_i X_i Y_i=0$

Minimum estimation variance

The estimation variance is

$$Var[Z^*(x_0)-Z(x)] = Var[\sum_{i=1}^{n}\lambda_i Z(x_i) - Z(x_0)]$$

Form equation 3.12, as is known, the estimation variance can be expressed as a quadratic form in λ_i, λ_j. Thus, the minimization of equation 3.12 subject to the unbiased constraints of equation 3.11 yields the "Kriging system "

$$\sum_{j=1}^{n}\lambda_j K(x_i-x_j) + \sum_{l=0}^{\nu}\mu_l f^l(x_i) = K(x_0-x_i) \qquad i=1,2,\ldots,n$$

$$\sum_{j=1}^{n}\lambda_j f^l(x_j) = f^l(x_0) \qquad l=0,1,\ldots,\nu$$

Its matrix form

$$\begin{bmatrix} K_{11} & K_{12} & \ldots & K_{1n} & 1 & f^1(x_1) & \ldots & f^\nu(x_1) \\ K_{21} & K_{22} & \ldots & K_{2n} & 1 & f^1(x_2) & \ldots & f^\nu(x_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ K_{n1} & K_{n2} & \ldots & K_{nn} & 1 & f^1(x_1) & \ldots & f^\nu(x_n) \\ 1 & 1 & \ldots & 1 & 0 & 0 & \ldots & 0 \\ f^1(x_1) & f^1(x_2) & \ldots & f^1(x_n) & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ f^\nu(x_1) & f^\nu(x_2) & \ldots & f^\nu(x_n) & 0 & 0 & \ldots & 0 \end{bmatrix} \times \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \\ \mu_0 \\ \mu_1 \\ \vdots \\ \mu_\nu \end{bmatrix} = \begin{bmatrix} K_{10} \\ K_{20} \\ \vdots \\ K_{n0} \\ 1 \\ f^1(x) \\ f^2(x) \\ \vdots \\ f^\nu(x) \end{bmatrix}$$

where $K_{ij} = Kx_i - x_j, K_{i0} = K(x_i - x)$

From the solution of the "Kriging system ", the variance of the estimation is derived

$$Var[\sum_{i=0}^{n}\lambda_i Z(x_i)] = K(0) - \sum_{l=0}^{\nu}\mu_l f^l(x_0) - \sum_{i=0}^{n}\lambda_i K(x_i - x_0)$$

The "Kriging system "shows that the knowledge of the generalized covariance $K(h)$ is the only prerequisite for the estimation process. In contrast to universal Kriging, the theory of intrinsic random function allows the generalized covariance $K(h)$ to be estimated directly. In the next chapter, the procedure of finding an optimal generalized covariance will be presented.

3.6 Other Related Kriging Methods: Lognormal Kriging, Cokriging, Disjunctive Kriging, Conditional Simulation

All the common types of Kriging technique have been described in the previous sections. This section will briefly describe the rest of Kriging related methods. Among these methods, some are complementary to the described Kriging methods while others are more advanced methods developed on the basis of Kriging. More detailed descriptions can be found in the references mentioned next.

Lognormal Kriging

One of the assumption of the theory of regionalized variables is the normality of data distribution. It is known that most phenomena in natural world present the characteristic of normal distribution. In practice, it may not be easy to ascertain the normality of data distribution due to insufficient data. With sufficient data, however, it may be found that some data are not normally distributed and may be better fitted by a lognormal distribution. In this case, lognormal Kriging can be applied. In this method, instead of kriging with variable Z, its logarithm $log(Z)$ is kriged. Lognormal Kriging is often used in the mining industry(Krige, 1978). The main reason to emphasise the normality of data set is that a better spatial structure is ensured, which may be reflected by a strongly correlated variogram or covariance.

Cokriging

For kriging estimations, the more data available, the more accurate estimations may be made. Therefore, if two or more variables measured in fields are correlated, it is better to consider them together. In particular, if one variable may not have been sampled sufficiently to provide reliable estimations, the precision of the estimation may then be improved by including the data of another correlated variable. Cokriging is a useful technique which can be used in the above case. For example, supposing that the concentration of dissolved oxygen and salinity sampled in estuaries are correlated, then more accurate estimations for dissolved oxygen can be made by using the cokriging method because dissolved oxygen data are usually insufficiently measured. Cokriging is similar to the usual Kriging methods. The general formulation of the method can be found in the following references(Journel, 1978; Marsily, 1986; Varlly, 1984)

Disjunctive Kriging

In ordinary Kriging where the second-order stationarity is satisfied, if the original data is or can be converted to Gaussian normal distribution, disjunctive Kriging may be used instead of ordinary Kriging. Disjunctive Kriging uses a nonlinear unbiased estimator and provides a better estimation than ordinary linear kriging(Journel, 1978; Guarasio, 1975; Yater, 1986). A major disadvantage in using disjunctive Kriging is that it is computationally more expensive.

Conditional Simulation

In kriging, the uncertainty of an estimation is expressed as the estimation variance from which 95% of the estimation confidence interval can be known. Therefore, the accuracy of an estimation can be assessed approximately, which is an improvement in comparison with other methods which have no indications for their estimation accuracy. However, if the uncertainty needs to be quantified, the Kriging technique is not applicable. Conditional simulation(Delhomme, 1979; Journal, 1978) is such a method designed to solve the uncertainty. Conditional simulation has the following properties:

(1) give the sampled values at the measurements points

(2) has the same distribution and structure as the sampled data

There are three distinctive steps in using conditional simulation. First step is to generate different realizations $Z_s(x)$ of the random function Z(x) with methods such as turning bands(Matheron, 1973) and spectral analysis(Mejia, 1974). The second step is to make simulation values equal to the sampled values at the sampled points. The final step is to determine the uncertainty or residual by appling the Kriging method.

Chapter 4 Application of Kriging

4.1 Introduction

The estuary of the River Tees in the north east of England is an estuary with pollution problems, and has been the subject of a number of large surveys since 1931. The purposes of those surveys were to characterize the estuary in terms of water quality and to provide data for water quality models.

In order to know the pollution level and determine parameters of a hydrodynamic or water quality model (e.g. dispersion coefficients), basic estuarine data such as velocity, salinity etc. are required. Thus, a survey of this kind aims to obtain reliable information from limited measurements. An insufficient number of sampling stations cannot meet the demands of data requirement, while a survey of many sampling stations is very expensive. Most surveying planners allocate sampling stations according to their experience or intuition. Hence, the crux of the above problem is how to find the minimum number of sampling stations which provide reliable data information.

Many surveys have been carried out on the River Tees. The earliest dated back to 1929 (Water Pollution Research Board, 1931). More frequent surveys have been performed since late 60's. For example, a survey was done in 1969 for the study of the hydrodynamics and pollution chemistry of the estuary. Estuary surveys may be carried out for a variety of purposes, e.g. hydrographical or chemical and may produce qualitative or quantitative data. The best application of Kriging is to survey data that need to be transformed into contoured plots.

A unique characteristic of Kriging is that it not only gives an estimation but provides an indication of estimation error. The variance of kriging estimations is a useful tool for optimizing a network of sampling stations because it does not directly include any measured values. Hence, additional points can be added to where the variances of estimation are high to find if these new points can decrease the variance of estimation effectively; meanwhile, existing measurement points can be left out to check if the variance of estimation is effected severely or not. In this way, new measurement points or stations can be found if necessary or unnecessary points can be detected.

This chapter attempts to solve the above stated problem by applying the Kriging technique. There are four sections in this chapter. First, the implementation of generalized Kriging will be described. Second, a 1-D case study will be reported to compare the results of cubic spline method with the kriging results. Third, a 2-D case study will investigate the allocation of sampling stations during 1975 survey on the River Tees. Finally, conclusions and discussions will be drawn from the above studies.

4.2 Implementation of Generalized Kriging

The sampled variables of a general estuarine survey vary from one station to another and even vary within one station. If a survey is performed in a vertical plane along the central axis of an estuary, those variables vary in both horizontal and vertical directions. For example, salinity decreases from an estuary mouth to its maximum limit of salt water penetration while it increases from the water surface to bottom. Other variables change in their particular trends as well. Those changes are often so irregular that traditional methods (least square approach, spline fit approach etc.) are difficult to apply. However, it may be seen that the characteristic of the sampled variables fits the definition of regionalized variables. Hence, the use of the Kriging method could be considered.

One of the three methods introduced in the section on the theory of Kriging must be chosen. Firstly, as the sampled variables have trends, the ordinary Kriging method which is suitable for the stationary case ought not to be used. Secondly, universal Kriging is applicable as long as the variogram $\gamma(h)$ is known, but it is still unusable with a variogram $\gamma(h)$ which can not be calculated from data. Thirdly, the application of the generalized Kriging method requires a known generalized covariance K(h) of order k. In contrast to the universal Kriging, the generalized covariance K(h) and its order k can be determined from data with the help of an automatic procedure developed in the program AKRIP (Kafritsas, etc.)

In practice, the most commonly applied form of generalized covariances is the polynomial one even though there are other admissible forms. Polynomials of the order 0, 1 and 2 are commonly used for most cases since higher orders are rarely needed. Table-4.1 summarizes those valid models.

Table-4.1 Models of Polynomial Generalized Covariances

(After Delfiner, 1976)

Trend	k	f^l in (X,Y)	Models of P. G. C.
Constant	0	1	$K(h) = a\delta + bh$
Linear	1	1, X, Y	$K(h) = a\delta + bh + ch^3$
Quadratic	2	1, X, Y, X , Y , XY	$K(h) = a\delta + bh + ch^3 + dh^5$
Constraints		$b \leq 0, d \leq 0$	
on the		$c \geq -\frac{10}{3}\sqrt{bd}$	
Coefficients		$\delta = 0, \ \ if \ \ h \neq 0$	$\delta = 1, \ \ if \ \ h = 0$

Although the form of a model of the generalized covariance is known, further specification is needed. This can be accomplished by the so-called "structure identification "as follows

(1) identification of the order k

(2) determination of the coefficients of the polynomial generalized covariances

(3) selection of the best polynomial generalized covariance

The program AKRIP was designed to solve the problem of the structure identification. It is a package of computing programs consisting of a main program and 16 subroutines. In terms of CPU time consumption, it is quite expensive to run such a package if many data points are used in the kriging process.

4.3 1-D Case Study

The objective of using Kriging in one dimensional case is to find if it is able to give better estimations than the commonly used cubic spline method. The direction of the one dimension is from the water bottom to water surface at a fixed sampling station. The original AKRIP program was written only for two dimensional estimation problems. Thus, it was modified for use in the one dimensional estimation problem. The set of data was taken from readings at station 4 - Smith's Dock at 8:30 on 10th August 1970, consisting of variables of Salinity, Dissolved Oxygen(DO), Temperature.

Surprisingly, the estimations by the two methods are almost same. The result comparisons are shown for velocity(Fig. 4.1), salinity(Fig. 4.2), DO(Fig. 4.3). From the theoretical point of view, Matheron(1980) demonstrated that the two methods are equivalent in the sense that any fitted curve obtained using spline functions can be identified with a fit obtained using Kriging and vice versa. But, Kriging provides an interpolation method which is more general and more powerful than spline interpolation. The commonly used spline functions like cubic spline are just particular cases of Kriging interpolators. Another close examination on spline and Kriging was given by Dubrule(1983).

The sampling design in this case is straightforward. It is of little significance to study the number and positions of sampling points. Computationally, Kriging makes the interpolation complicated while the cubic spline method is simple and effective.

4.4 2-D Case Study

The 6 sets of the data analysed in this case were taken from the 1975 survey. In this survey, the observations were made over the periods 2-6 July 1975 and 9-13 July 1975 on neap tides and spring tides respectively, and the measurements of water depth, current speed and direction, salinity, temperature and percentage of dissolved oxygen were recorded simultaneously at half-hourly interval over a full tidal cycle on each day at eight stations along the central axis of the estuary(Fig. 7.1). The 6 sets of the data were the measurements at high water, mid tide and low water on 5 July 1975 and 12 July 1975 respectively so that they represented measurements at different times of different types of tides.

At each sampling station, the number of measured points between the surface and bottom varied with the depth. There were usually at least 8 points taken evenly over the depth which were regarded as sufficient to adequately define the profiles of the measured variables. Each sampling station was believed to

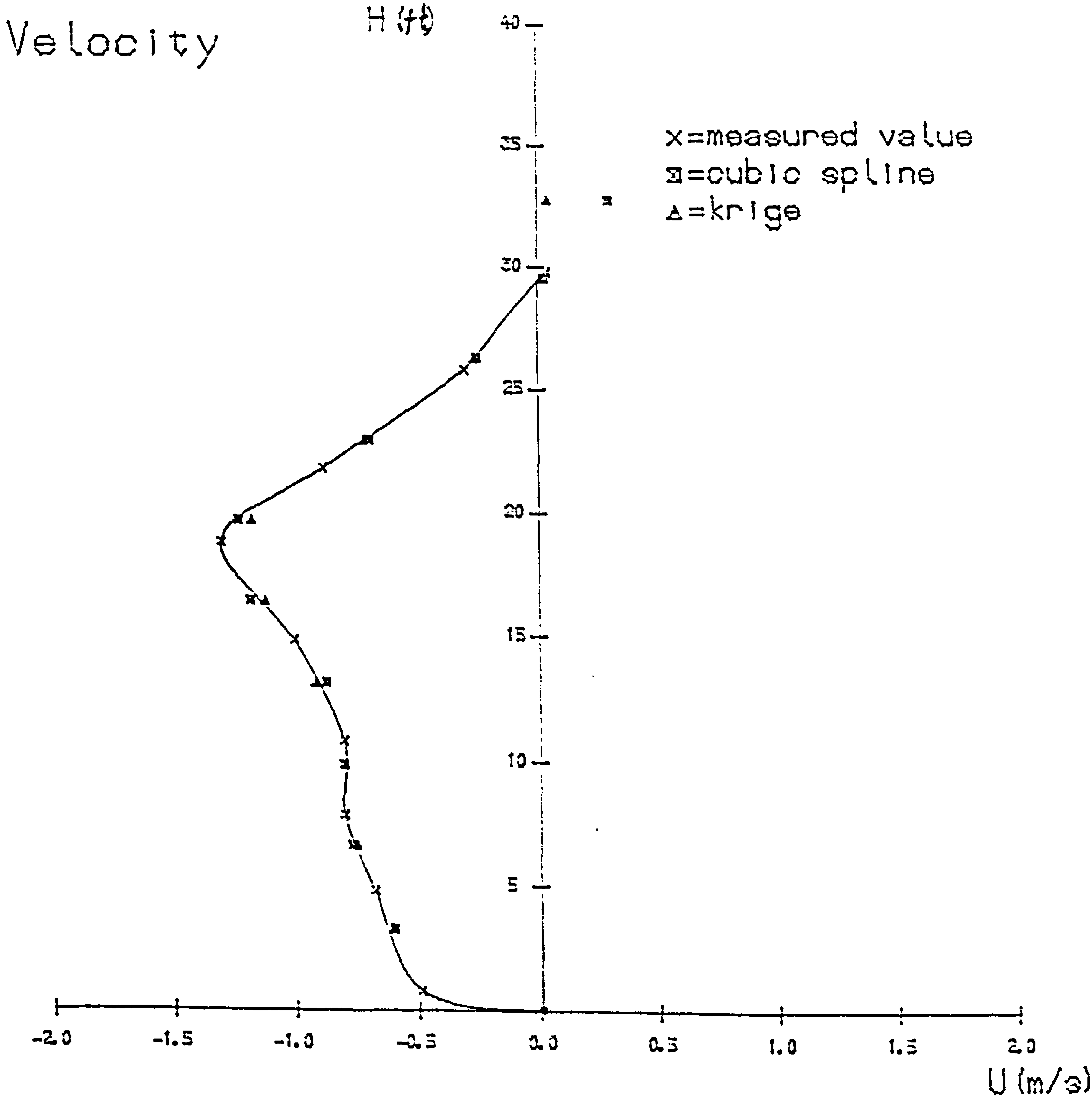

Fig. 4.1 Comparison between spline estimations and kriging estimations for velocity measurements

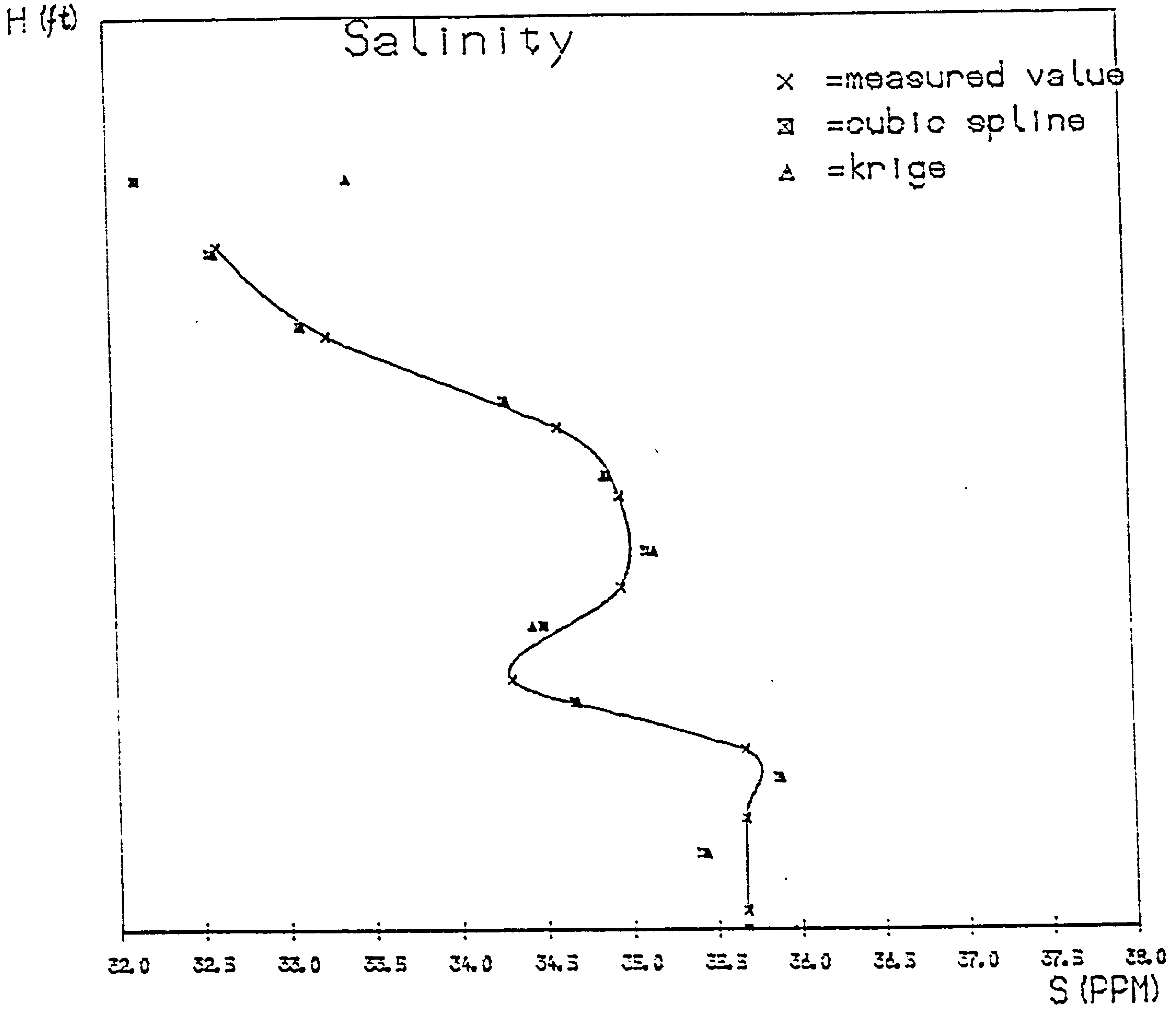

Fig. 4.2 Comparison between spline estimations and kriging estimations for salinity measurements

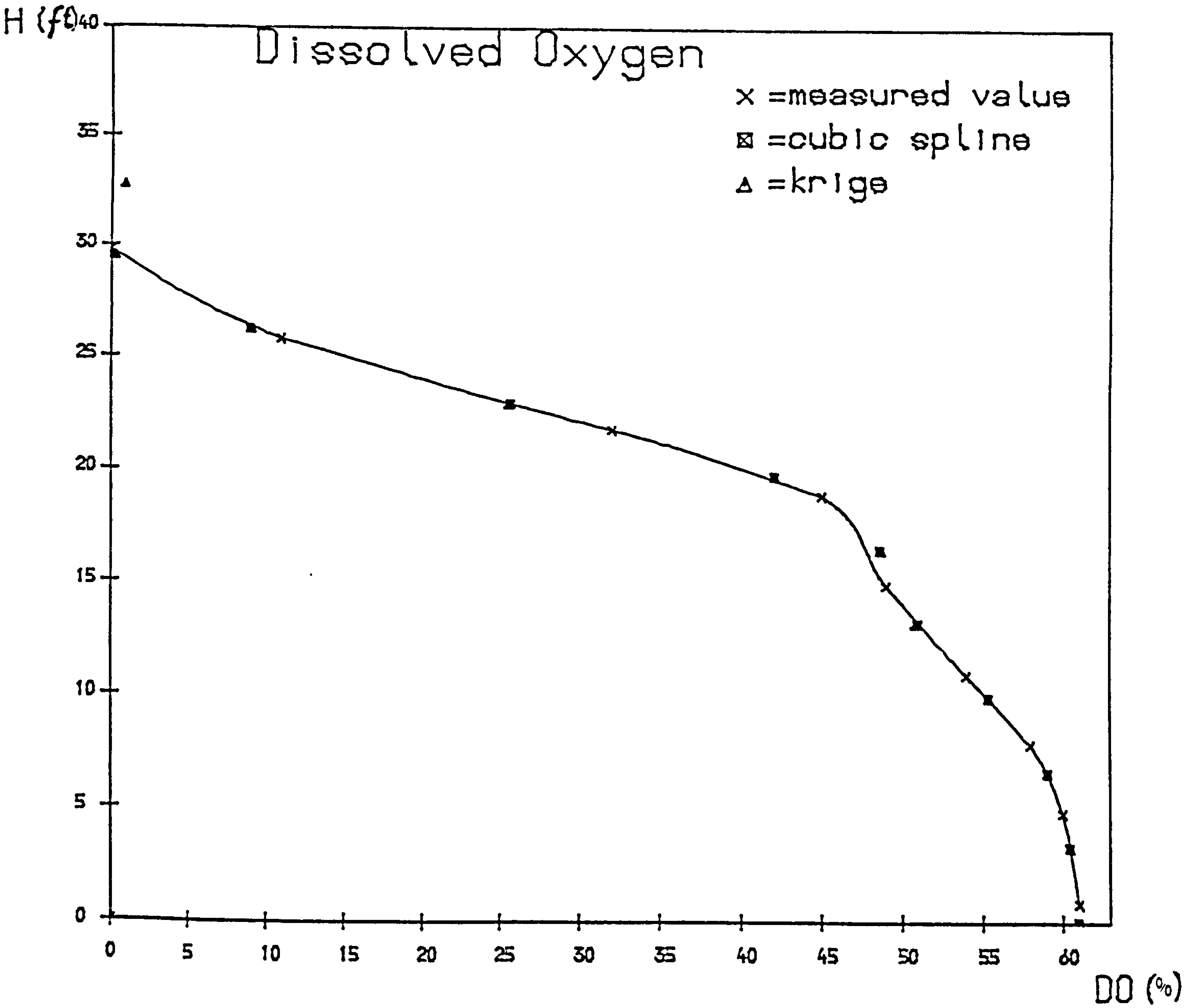

Fig. 4.3 Comparison between spline estimations and kriging estimations for DO measurements

provide an equal representation of measured variables at its location.

It is of importance for a survey planner to know the significance of each individual station and to identify possible redundant stations. In fact, the two problems are closely related since only less significant stations can be redundant ones. Thus, the first problem must be solved before the second one.

The criterion adopted in this analysis is the change in overall variance of the estimated parameters when a station was omitted. With all the 8 stations, the averaged variance should be minimum. The averaged variance is increased when one of the stations is omitted. Clearly, the bigger the increased variance, the more significant the missing station is. The computation of the above procedure was carried out with a modified form of the program AKRIP.

The procedure of re-estimation can then be used. The procedure is to estimate the measurements at the missing stations by the Kriging method using data from the other remaining stations. If the differences between the original measurements and re-estimations are small, the stations are said to be reproduceable. This means that the stations are redundant. The number of stations that can be eliminated in this way can only be identified by testing combinations of those less significant stations.

The last problem inhibiting Kriging applications is the scale of the X, Y coordinates. The X coordinate is defined as the one originating seawards from station 8 along the central axis of the estuary and the Y coordinate is defined as the one originating downwards from water surface. Thus, the scale ratio of X/Y is 1000. When such X, Y coordinates of measured points were input for the Kriging computations, unreasonably large coefficients of generalized covariances were calculated. The scale of X coordinate was subsequently reduced to the same scale as the Y coordinate and then reasonable generalized covariances were derived(Table-4.2, 4.3). The scale problem does not appear to have received attentions from other Kriging users who have generally studied cases with an equal scale of X, Y coordinates. Evidently, it is vital for users encountering scale problems to realize that the coordinate reduction may make the Kriging method applicable.

From the computations of using the 6 sets of data, the following conclusions with discussions are given:

(1) None of the 8 sampling stations is reproduceable for the measurements of velocity and dissolved oxygen as values of two variables are very erratic. Hence, more than 8 stations are recommended to produce more accurate estimations. As Kriging estimations rely on measurements, the accuracy can only be as good as the data permit.

(2) There are 4, 3, 2 stations reproduceable at high water, mid tide and low water respectively for the measurements of salinity. The errors of the re-estimations are mostly less than 5% of measured values.(Fig. 4.4-4.12, Table-4.4)

(3) There are 4 stations reproduceable at high water, mid tide and low water for the measurements of temperature. The errors of the re-estimations are generally smaller than the errors of the re-estimations of salinity.(Fig. 4.13-4.24, Table-4.5)

(4) From the test of significance on salinity measurements, stations 8 and 7 are of most significance, and then stations 1 and 2 are of importance. The rest stations 3, 4, 5, 6 are of less significance. Because station 8 and 7 are located at the part of abrupt change of salinity near the upstream end and stations 1 and 2 are located near seawards end, they should be more important than the other stations. This conforms to Lewis's suggestion of selecting sampling stations to span the region of the maximum longitudinal salinity gradient(R.E.

Lewis's personal correspondence with D.J. Elliott, May, 1986). However, the observed salinity values at station 1 and 2 were close to each other, the predicted importance of station 2 was contradictory to general sense. As to this anomaly, there is no apparent explanation. In general, the test of significance provided both logical and reasonable assessments. If a new station is added, it should be positioned in the region of the most significant stations.

In the above study, the maximal combinations of stations were obtained through trial and error starting from combinations of fewer stations. For each combination of stations, differences between Kriged and observed values were checked for selecting a combination with smaller differences. At the end of this part of study, it is necessary to stress the problem of station reproducibility. As was mentioned in the procedure of re-estimation, stations are said to be reproduceable if the differences between the original measurements and re-estimations are small. Here, the word "small" is very vague, thus quantitative criteria ought to be used to judge reproducibility. Ideally, the criteria to judge measurement errors in form of either percentage of the measured values or deviation range of the measured values should be adapted as the criteria to judge reproducibility. If the differences between the original measurements and re-estimations satisfy such a criterion, stations could be said reproduceable in terms of measurement errors. However, it remained a problem how to quantify the measurement errors from the raw data supplied as no information about the accuracy of instruments operated during the survey was available. An effort was made to try to find the information about the measurement errors in the published research papers on the river Tees. It was found the required information was not described in these papers either. As a result of this factor, the differences between measurements and re-estimations could not be compared with estimates of measurement errors. For further study, it would be desirable to carry out the comparision when the information of measurement errors become available.

From this study, the Kriging method, in particular, the generalized method, has been shown as a potential tool for the planners who need economical and scientific guidelines for expensive surveys. However, the exploitation of the method is extensive. The Kriging method will be incorporated with estuarine water quality models to provide velocity data.

Variable	Time	Order of drift, k	C	A1	A3	A5
Salinity	HW	2	-	-0.16734	-	-
	MW	2	-	-0.11204	-	-
	LW	2	-	-	0.013931	-
Velocity	HW	2	0.0016088	-0.00029495	-	-
	MW	2	-	-0.0036078	-	-
	LW	2	0.00048821	-0.0014526	-	-
Dissolved Oxygen	HW	2	-	-0.33403	-	-
	MW	2	-	-0.20111	-	-
	LW	2	-	-0.21468	-	-

$$K(h) = C\delta + A1h + A3h^3 + A5h^5$$

Table 4.2 Structure Identification Results: Parameters of Polynomial G.C. for Data from 5 July, 1975

Variable	Time	Order of drift, k	C	A1	A3	A5
Salinity	HW	2	-	-0.13756	-	-
	MW	2	-	-0.10427	-	-
	LW	2	-	-0.30858	-	-
Velocity	HW	2	-	-0.00071007	-	-
	MW	2	-	-0.026151	-	-0.0000018
	LW	2	-	−0.010199	-	-
Dissolved Oxygen	HW	2	-	-0.10086	-	-
	MW	1	-	-0.028556	-	-
	LW	1	-	-0.078842	-	-

$$K(h) = C\delta + A1h + A3h^3 + A5h^5$$

Table 4.3 Structure Identification Results: Parameters of Polynomial G.C. for Data from 12 July, 1975

TABLE 4.4 COMPARISIONS BETWEEN MEASUREMENTS AND RE-ESTIMATIONS FOR SALINITY
AT STATIONS 7, 5, 3, 2 (X=4.0, 9.3, 13.7, 16.1 km) DURING HIGH WATER
AT STATIONS 5, 4, 2 (X=9.3, 11.3, 16.1 km) DURING MIDDLE WATER
AT STATIONS 4, 2 (X=11.3, 16.1 km) DURING LOW WATER

High Water (7:00 hr 12 July 1975)

X (km)	Y (m)	z (ppm)	z* (ppm)	z*-z (ppm)	|z*-z|/z (%)
4.00	0.25	27.40	28.74	1.34	4.90
4.00	1.00	27.50	29.03	1.53	5.57
4.00	2.00	29.00	29.53	0.53	1.84
4.00	3.00	30.20	30.10	-0.10	0.32
4.00	4.00	30.70	30.64	-0.06	0.19
4.00	5.00	31.50	31.07	-0.43	1.35
4.00	6.00	31.90	31.38	-0.52	1.64
9.30	0.25	30.50	31.22	0.72	2.36
9.30	1.00	31.00	31.41	0.41	1.32
9.30	2.00	31.25	31.75	0.50	1.60
9.30	3.00	31.50	32.13	0.63	2.01
9.30	4.00	31.75	32.48	0.73	2.29
9.30	5.00	32.00	32.75	0.75	2.34
9.30	6.00	32.00	32.93	0.93	2.90
9.30	7.00	32.00	33.01	1.01	3.16
9.30	8.00	32.00	33.04	1.04	3.25
9.30	9.00	32.00	33.05	1.05	3.28
9.30	10.00	32.10	33.05	0.95	2.96
9.30	11.00	32.10	33.04	0.94	2.93
9.30	12.00	32.10	33.02	0.92	2.87
13.70	0.25	30.10	32.93	2.83	9.40
13.70	2.00	32.80	33.03	0.23	0.69
13.70	4.00	33.10	33.12	0.02	0.06
13.70	6.00	33.50	33.20	-0.30	0.88
13.70	8.00	33.55	33.19	-0.36	1.08
13.70	10.00	33.55	33.21	-0.34	1.01
13.70	12.00	33.55	33.32	-0.23	0.69
13.70	14.00	33.60	33.45	-0.15	0.43
16.10	0.25	33.80	33.71	-0.09	0.27
16.10	2.00	33.95	33.75	-0.20	0.59
16.10	4.00	34.00	33.77	-0.23	0.67
16.10	6.00	34.05	33.78	-0.27	0.80
16.10	8.00	34.06	33.78	-0.28	0.81
16.10	10.00	34.10	33.81	-0.29	0.85
16.10	12.00	34.21	33.89	-0.32	0.95
16.10	14.00	34.35	33.97	-0.38	1.09
16.10	16.00	34.35	34.05	-0.30	0.88

Middle Water (10:00 hr 12 July 1975)

X (km)	Y (m)	z (ppm)	z* (ppm)	z*-z (ppm)	|z*-z|/z (%)
9.30	0.25	28.50	30.46	1.96	6.87
9.30	1.00	29.00	30.58	1.58	5.45
9.30	2.00	29.20	30.85	1.65	5.66
9.30	3.00	29.60	31.25	1.65	5.58
9.30	4.00	29.75	31.70	1.95	6.54
9.30	5.00	30.00	32.09	2.09	6.98
9.30	6.00	30.30	32.41	2.11	6.98
9.30	7.00	30.80	32.67	1.87	6.07
9.30	8.00	31.00	32.83	1.83	5.91
9.30	9.00	31.50	32.87	1.37	4.34
9.30	10.00	31.60	32.83	1.23	3.88
11.30	0.25	31.00	31.70	0.70	2.27
11.30	1.00	31.00	31.77	0.77	2.47
11.30	2.00	31.10	31.92	0.82	2.64
11.30	3.00	31.30	32.14	0.84	2.68
11.30	4.00	31.60	32.39	0.79	2.50
11.30	5.00	32.00	32.64	0.64	1.99
11.30	6.00	32.45	32.85	0.40	1.24
11.30	7.00	32.63	33.02	0.39	1.21
11.30	8.00	32.65	33.15	0.50	1.54
16.10	0.25	32.56	33.60	1.04	3.19
16.10	2.00	33.20	33.69	0.49	1.49
16.10	4.00	33.55	33.87	0.32	0.95
16.10	6.00	33.91	34.00	0.09	0.26
16.10	8.00	34.11	34.09	-0.02	0.06
16.10	10.00	34.22	34.30	0.08	0.22
16.10	12.00	34.24	34.69	0.45	1.32
16.10	14.00	34.24	35.05	0.81	2.36
16.10	16.00	34.25	35.26	1.01	2.96

z = measurements

z*= re-estimations

Low Water (13:00 hr 12 July 1975)

X (km)	Y (m)	z (ppm)	z* (ppm)	z*-z (ppm)	|z*-z|/z (%)
11.3	0.25	28.50	26.57	-1.93	6.78
11.3	1.00	28.50	27.29	-1.21	4.23
11.3	2.00	28.70	28.17	-0.53	1.84
11.3	3.00	29.20	29.00	-0.20	0.70
11.3	4.00	30.10	29.71	-0.39	1.31
11.3	5.00	31.10	30.34	-0.76	2.44
11.3	6.00	31.70	30.93	-0.77	2.43
16.1	0.25	33.00	31.19	-1.81	5.49
16.1	2.00	33.00	31.56	-1.41	4.35
16.1	4.00	33.45	31.99	-1.46	4.35
16.1	6.00	33.80	32.44	-1.40	4.13
16.1	8.00	34.03	32.71	-1.32	3.87
16.1	10.00	34.13	33.14	-0.99	2.91
16.1	12.00	34.17	33.83	-0.34	0.99
16.1	14.00	34.25	34.45	0.20	0.58

TABLE 4.5 COMPARISIONS BETWEEN MEASUREMENTS AND RE-ESTIMATIONS FOR TEMPERATURES AT STATIONS 7(X=4.0 km), 5(X=9.3 km), 4(X=11.3 km), 2(X=16.1 km)

High Water (7:00 hr 12 July 1975)

X (km)	Y (m)	z (°C)	z* (°C)	z*-z (°C)	|z*-z|/z (%)
4.00	0.25	17.60	16.38	-1.22	6.92
4.00	1.00	17.60	16.28	-1.32	7.50
4.00	2.00	17.20	16.14	-1.06	6.15
4.00	3.00	16.40	15.99	-0.41	2.49
4.00	4.00	16.20	15.84	-0.36	2.24
4.00	5.00	15.70	15.70	-0.00	0.00
4.00	6.00	15.40	15.59	0.19	1.23
9.30	0.25	15.00	15.30	0.73	4.86
9.30	1.00	14.80	15.50	0.70	4.75
9.30	2.00	14.60	15.21	0.61	4.19
9.30	3.00	14.60	14.93	0.33	2.23
9.30	4.00	14.30	14.67	0.37	2.56
9.30	5.00	14.20	14.46	0.26	1.81
9.30	6.00	14.10	14.30	0.20	1.44
9.30	7.00	14.00	14.19	0.19	1.38
9.30	8.00	14.00	14.11	0.11	0.82
9.30	9.00	14.00	14.06	0.06	0.42
9.30	10.00	14.00	14.02	0.02	0.13
9.30	11.00	13.90	13.99	0.09	0.67
9.30	12.00	13.90	13.99	0.09	0.62
11.30	0.25	14.70	15.70	1.00	6.80
11.30	1.00	14.65	15.38	0.73	5.01
11.30	2.00	14.50	14.99	0.49	3.37
11.30	3.00	14.40	14.67	0.27	1.85
11.30	4.00	14.25	14.42	0.17	1.17
11.30	5.00	14.00	14.21	0.21	1.52
11.30	6.00	13.90	14.05	0.15	1.09
11.30	7.00	13.90	13.94	0.04	0.27
11.30	8.00	13.80	13.86	0.06	0.45
11.30	9.00	13.80	13.81	0.01	0.10
11.30	10.00	13.80	13.78	-0.02	0.12
11.30	11.00	13.80	13.77	-0.03	0.23
16.10	0.25	14.00	14.62	0.62	4.46
16.10	2.00	13.80	14.10	0.30	2.17
16.10	4.00	13.80	13.82	0.02	0.12
16.10	6.00	13.60	13.65	0.05	0.40
16.10	8.00	13.60	13.55	-0.05	0.35
16.10	10.00	13.50	13.47	-0.03	0.20
16.10	12.00	13.20	13.36	0.16	1.25
16.10	14.00	13.00	13.26	0.26	1.97
16.10	16.00	13.00	13.20	0.20	1.54

Middle Water (10:00 hr 12 July 1975)

X (km)	Y (m)	z (°C)	z* (°C)	z*-z (°C)	|z*-z|/z (%)
4.0	0.25	19.40	17.82	-1.58	8.17
4.0	1.00	19.40	17.71	-1.69	8.72
4.0	2.00	19.40	17.56	-1.84	9.48
4.0	3.00	19.40	17.40	-2.00	10.29
9.3	0.25	16.80	15.94	-0.86	5.09
9.3	1.00	16.20	15.85	-0.35	2.17
9.3	2.00	16.20	15.71	-0.49	3.04
9.3	3.00	15.80	15.55	-0.25	1.59
9.3	4.00	15.80	15.38	-0.42	2.64
9.3	5.00	15.60	15.22	-0.38	2.40
9.3	6.00	15.40	15.08	-0.32	2.05
9.3	7.00	15.20	14.96	-0.24	1.57
9.3	8.00	15.00	14.85	-0.15	0.97
9.3	9.00	14.70	14.76	0.06	0.40
9.3	10.00	14.60	14.67	0.07	0.50
11.3	0.25	15.90	15.33	-0.57	3.62
11.3	1.00	.15.70	15.23	-0.47	3.00
11.3	2.00	15.50	15.10	-0.40	2.58
11.3	3.00	15.40	14.97	-0.43	2.80
11.3	4.00	15.10	14.84	-0.26	1.74
11.3	5.00	14.80	14.71	-0.09	0.60
11.3	6.00	14.40	14.60	0.20	1.36
11.3	7.00	14.30	14.49	0.19	1.35
11.3	8.00	14.30	14.40	0.10	0.71
16.1	0.25	15.40	14.48	-0.92	6.00
16.1	2.00	14.80	14.29	-0.51	3.48
16.1	4.00	14.30	14.08	-0.22	1.55
16.1	6.00	13.80	13.91	0.11	0.83
16.1	8.00	13.50	13.80	0.30	2.19
16.1	10.00	13.30	13.70	0.40	2.97
16.1	12.00	13.30	13.60	0.30	2.23
16.1	14.00	13.20	13.50	0.30	2.31
16.1	16.00	13.20	13.47	0.23	1.72

z = measurements

z*= re-estimations

Low Water (13:00 hr 12 July 1975)

X (km)	Y (m)	z (°C)	z* (°C)	z*-z (°C)	|z*-z|/z (%)
4.0	0.25	20.20	19.54	-0.66	3.27
4.0	1.00	20.20	19.43	-0.77	3.81
9.3	0.25	18.40	18.17	-0.23	1.25
9.3	1.00	18.00	18.03	0.03	0.16
9.3	2.00	17.80	17.77	-0.03	0.19
9.3	3.00	16.80	17.44	0.64	3.83
9.3	4.00	16.40	17.08	0.68	4.15
9.3	5.00	16.20	16.69	0.49	3.01
9.3	6.00	15.20	16.30	1.10	7.24
9.3	7.00	14.80	15.96	1.16	7.83
11.3	0.25	16.90	17.04	0.14	0.85
11.3	1.00	16.90	16.84	-0.06	0.38
11.3	2.00	16.70	16.54	-0.06	0.93
11.3	3.00	16.40	16.24	-0.06	0.98
11.3	4.00	15.90	15.93	0.03	0.18
11.3	5.00	15.30	15.62	0.32	2.10
11.3	6.00	14.90	15.34	0.44	2.93
16.1	0.25	15.00	15.39	0.39	2.61
16.1	2.00	15.00	15.00	0.00	0.01
16.1	4.00	14.40	14.63	0.23	1.61
16.1	6.00	14.00	14.31	0.31	2.23
16.1	8.00	13.70	13.97	0.27	1.96
16.1	10.00	13.50	13.71	0.21	1.53
16.1	12.00	13.40	13.54	0.14	1.04
16.1	14.00	13.20	13.30	0.10	0.78

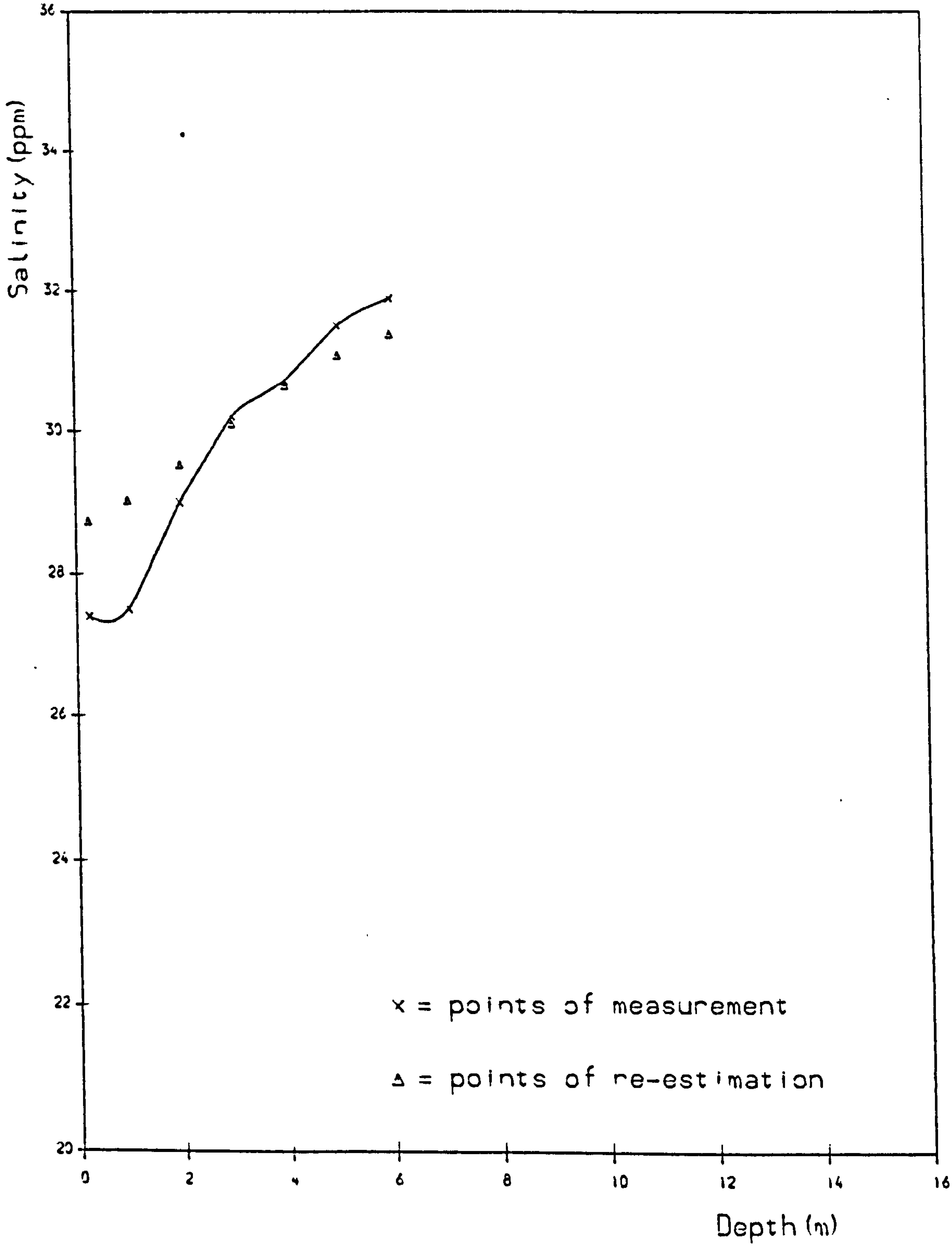

Fig. 4.4 Comparison between measurements and re-estimations

station 7 High Water

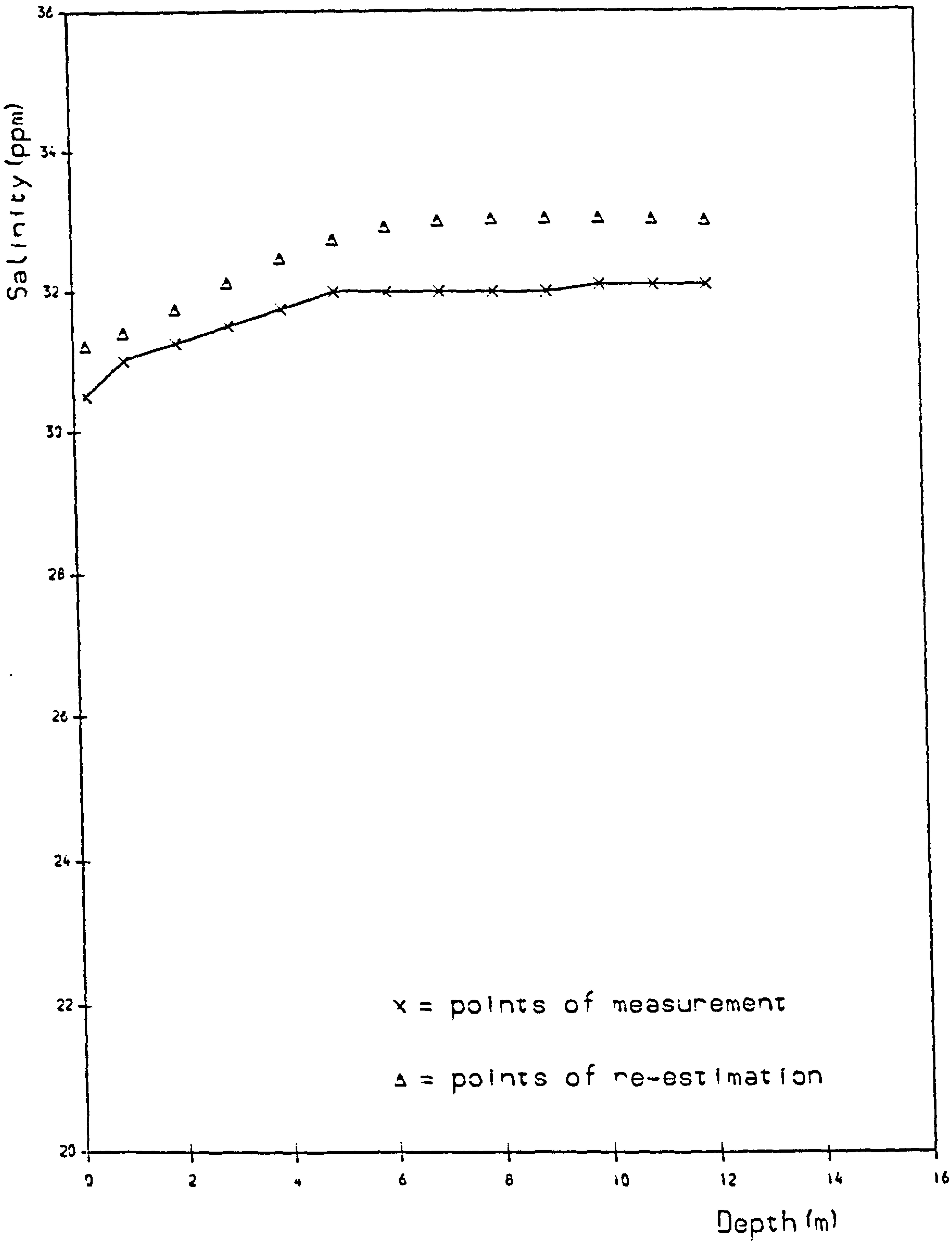

Fig. 4.5 Comparison between measurements and re-estimations

station 5 High Water

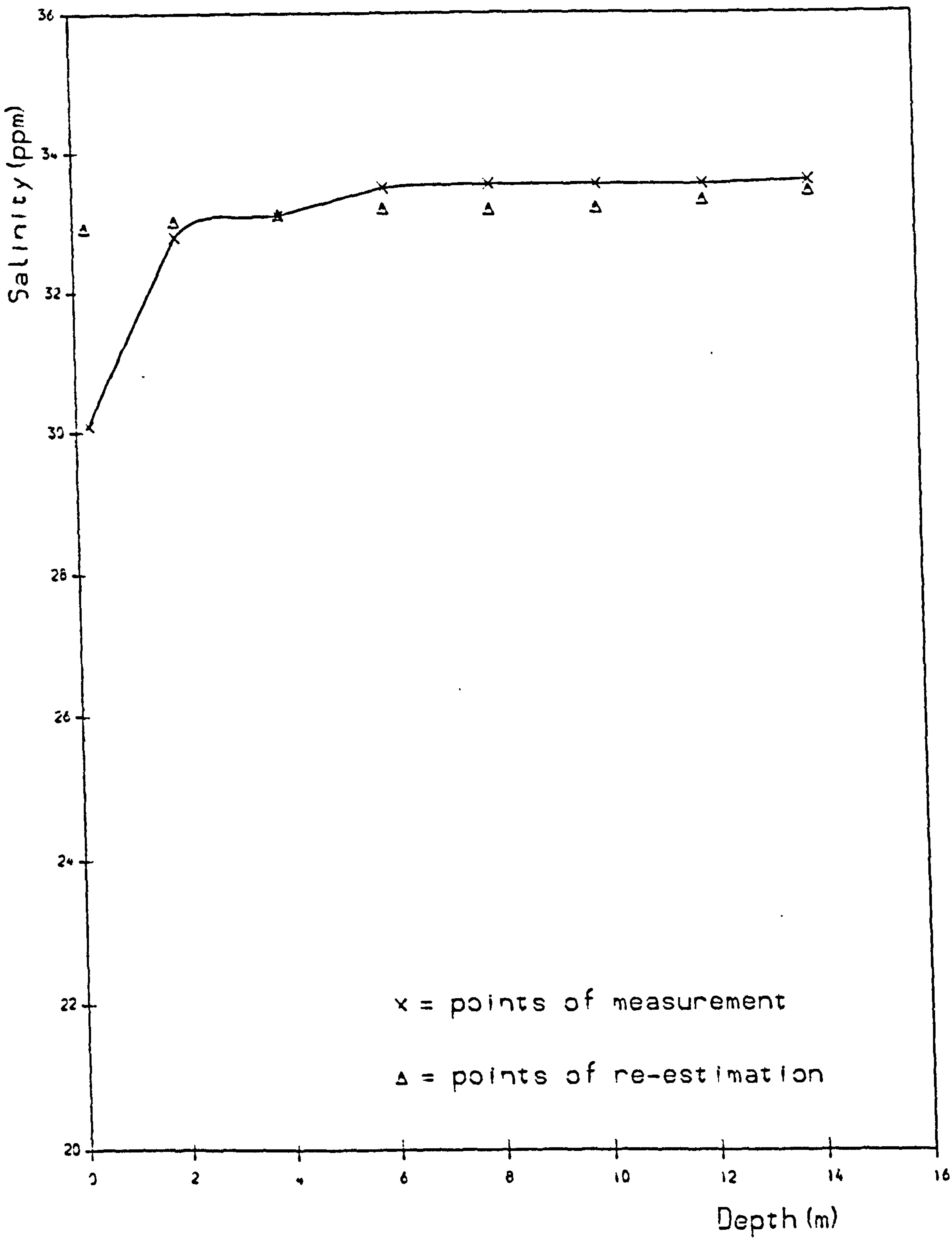

Fig. 4.6 Comparison between measurements and re-estimations

station 3 High Water

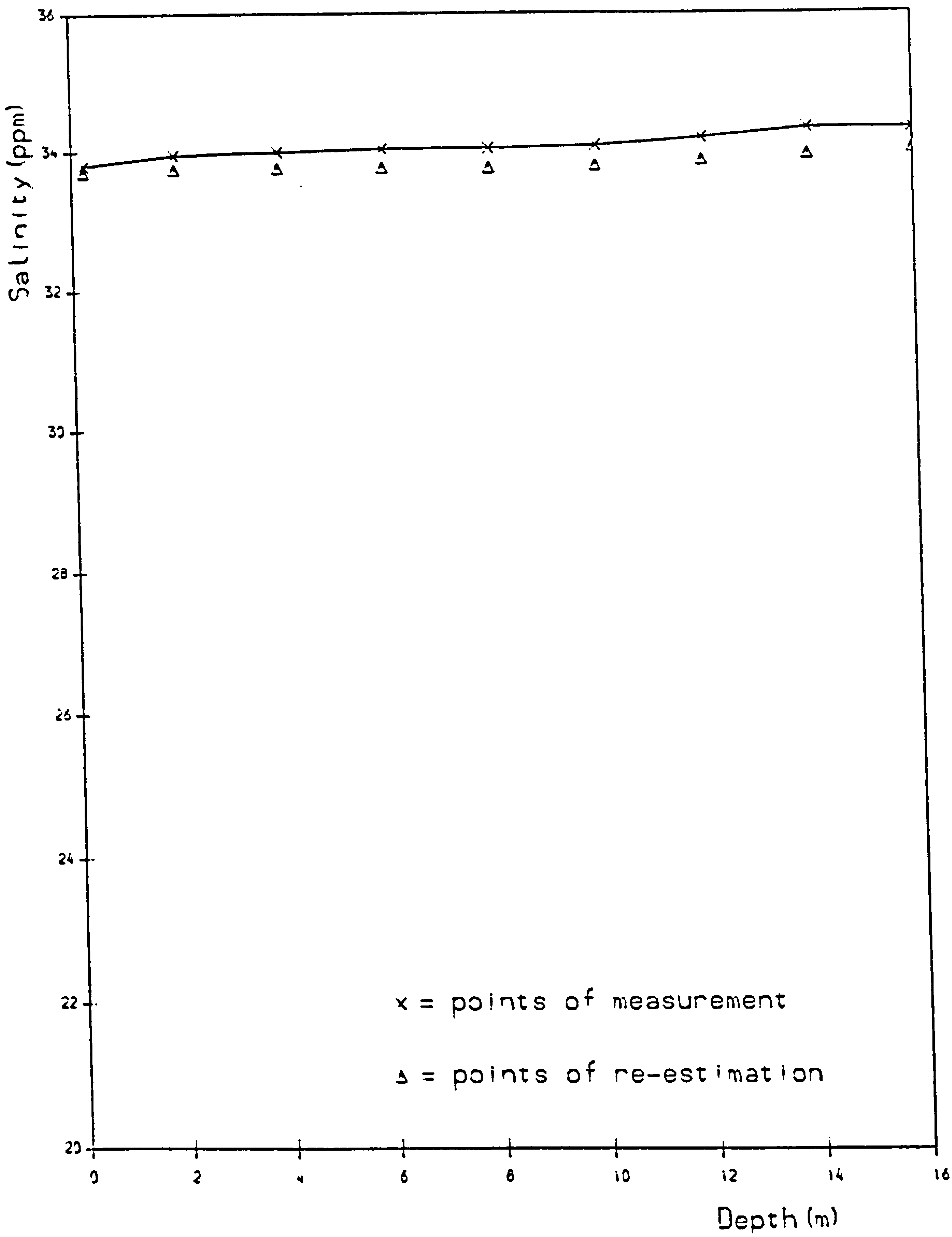

Fig. 4.7 Comparison between measurements and re-estimations

station 2 High Water

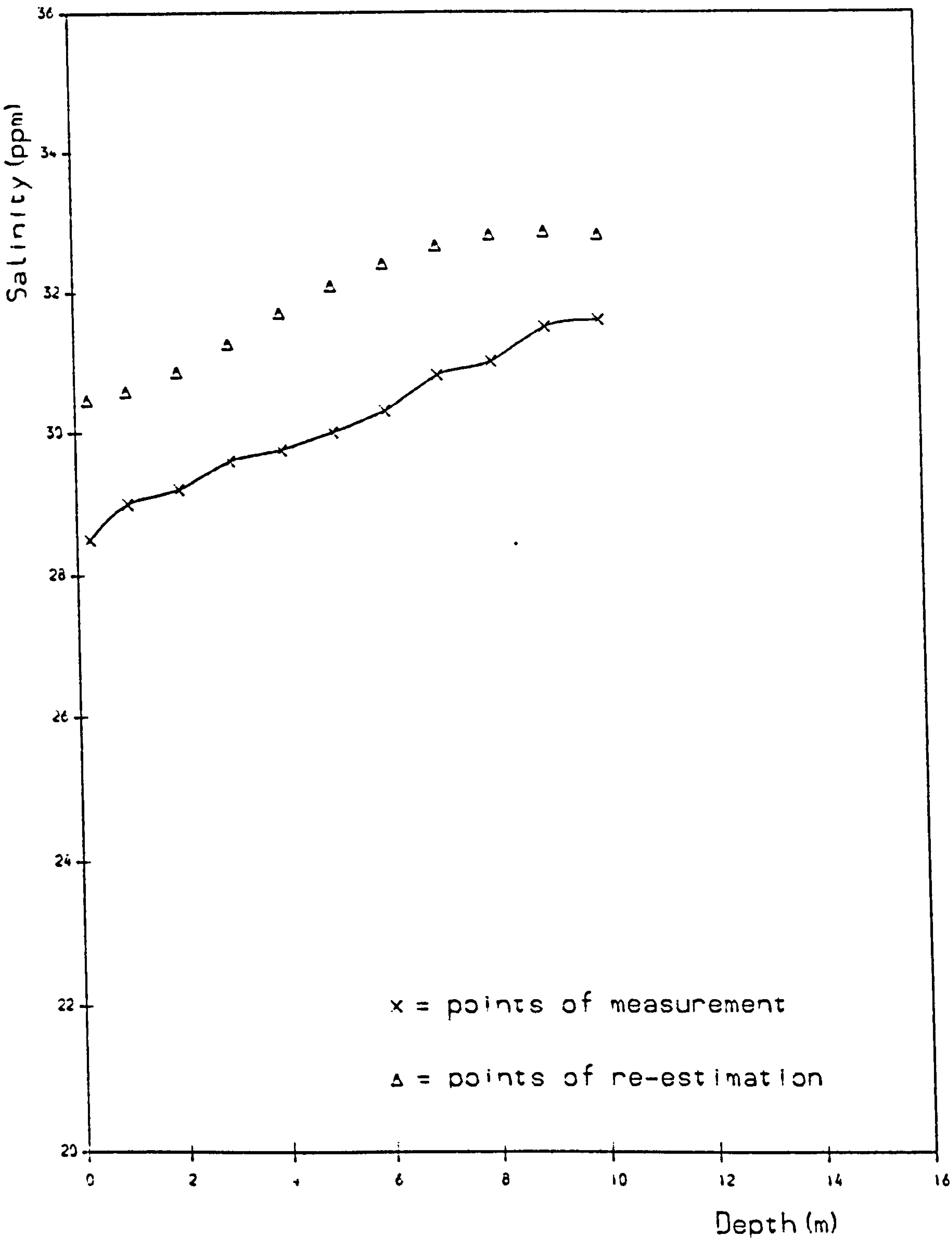

Fig. 4.8 Comparison between measurements and re-estimations

station 5 Mid Tide

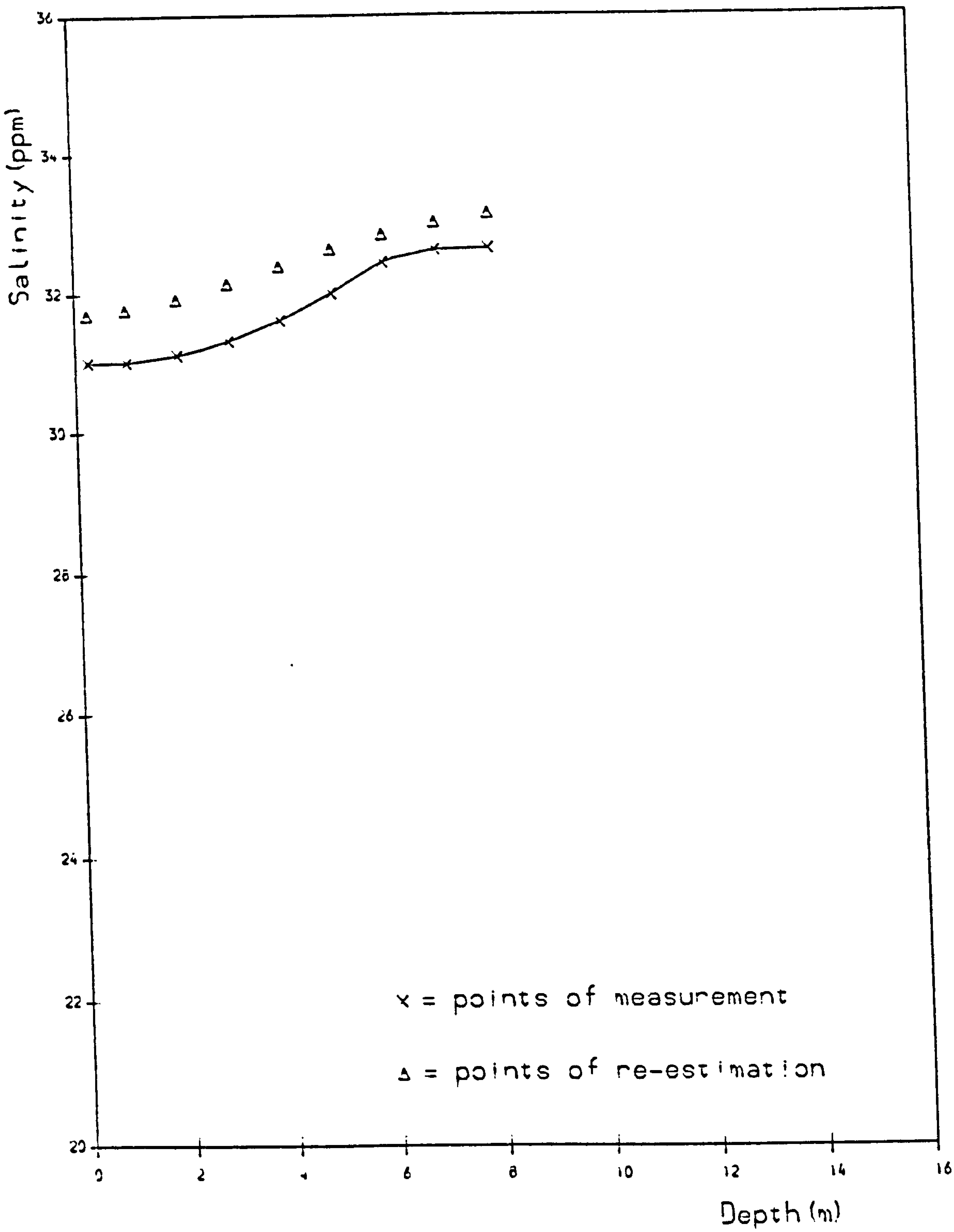

Fig. 4.9 Comparison between measurements and re-estimations station 4 Mid Tide

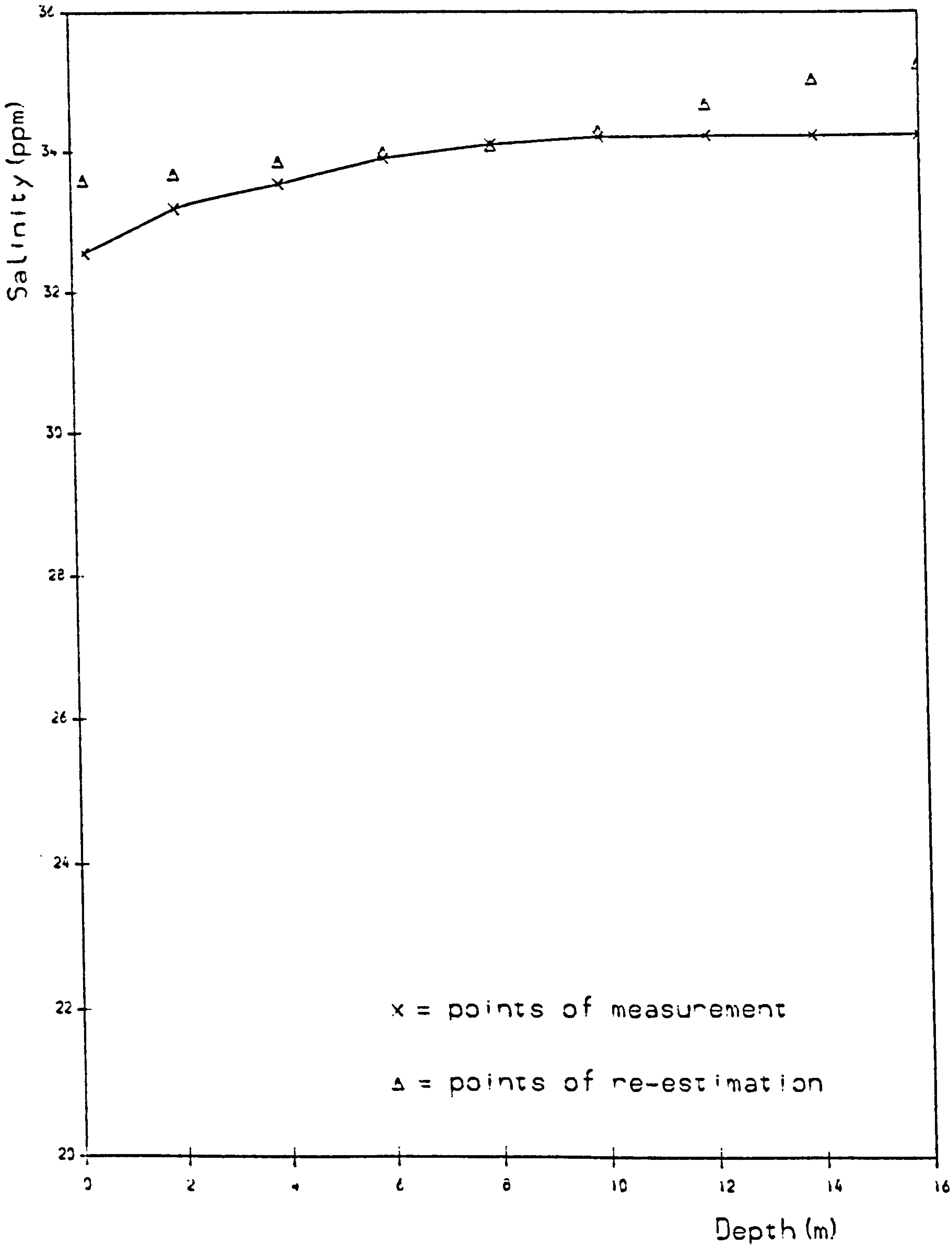

Fig. 4.10 Comparison between measurements and re-estimations
station 2 Mid Tide

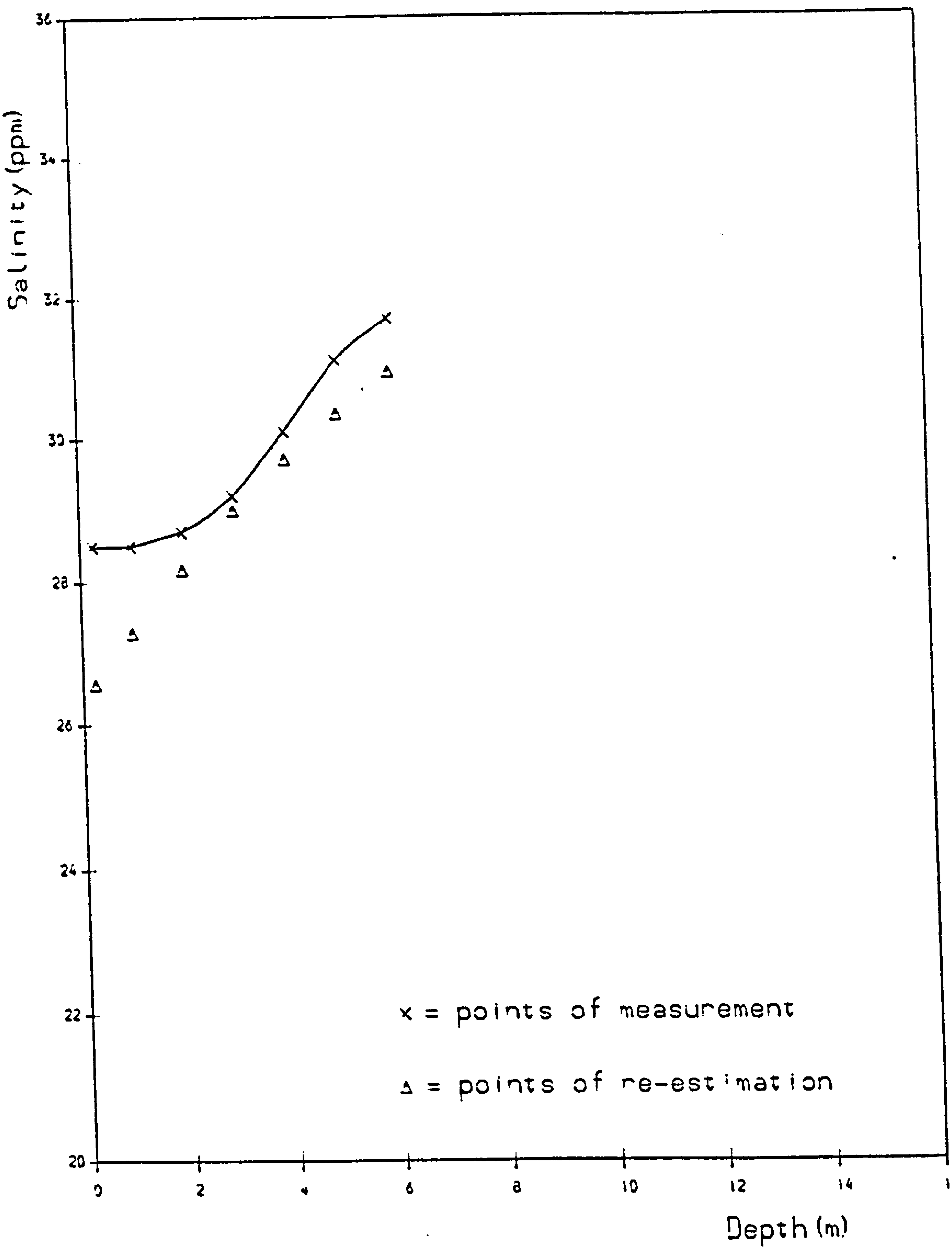

Fig. 4.11 Comparison between measurements and re-estimations

station 4 Low Water

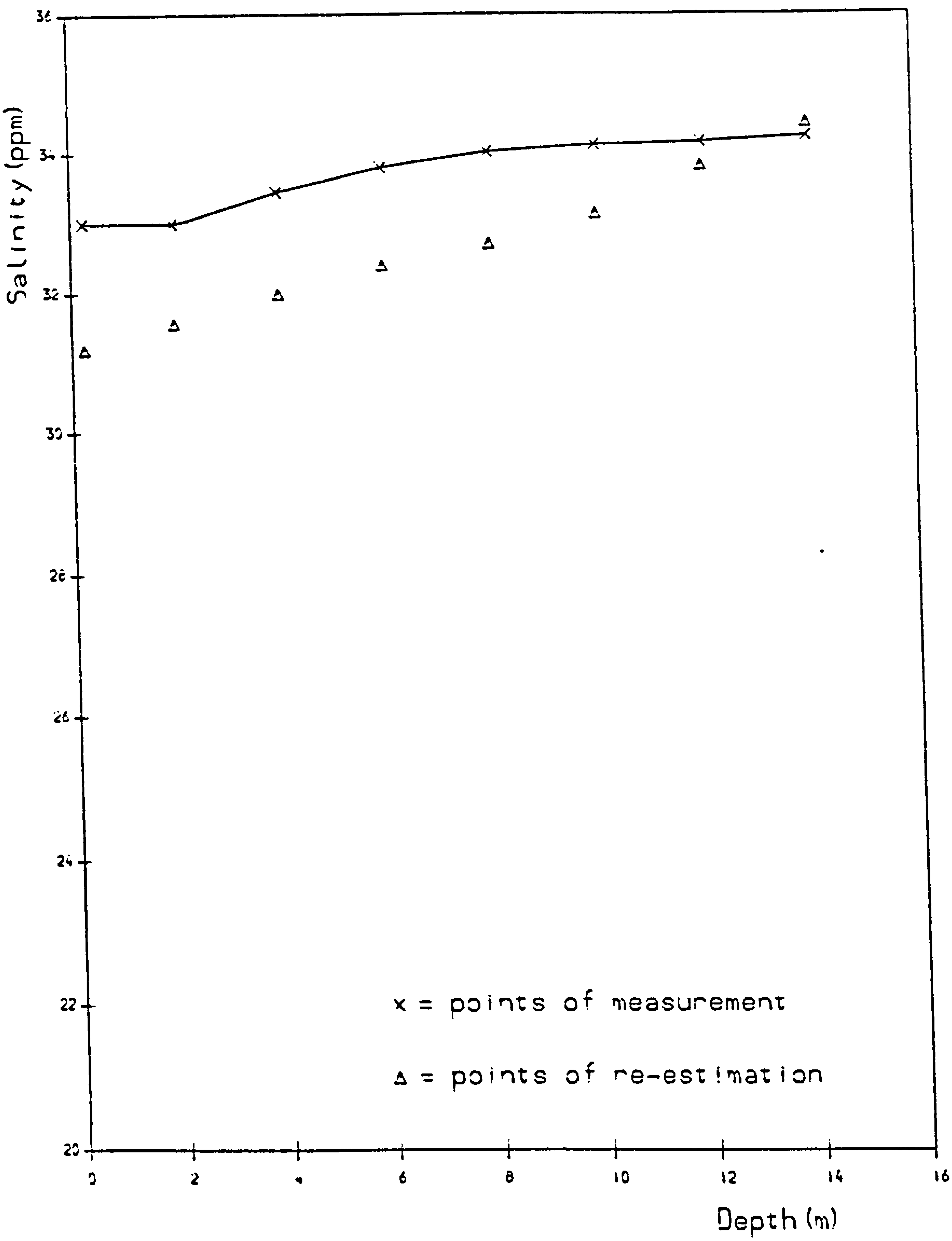

Fig. 4.12 Comparison between measurements and re-estimations

station 2 Low Water

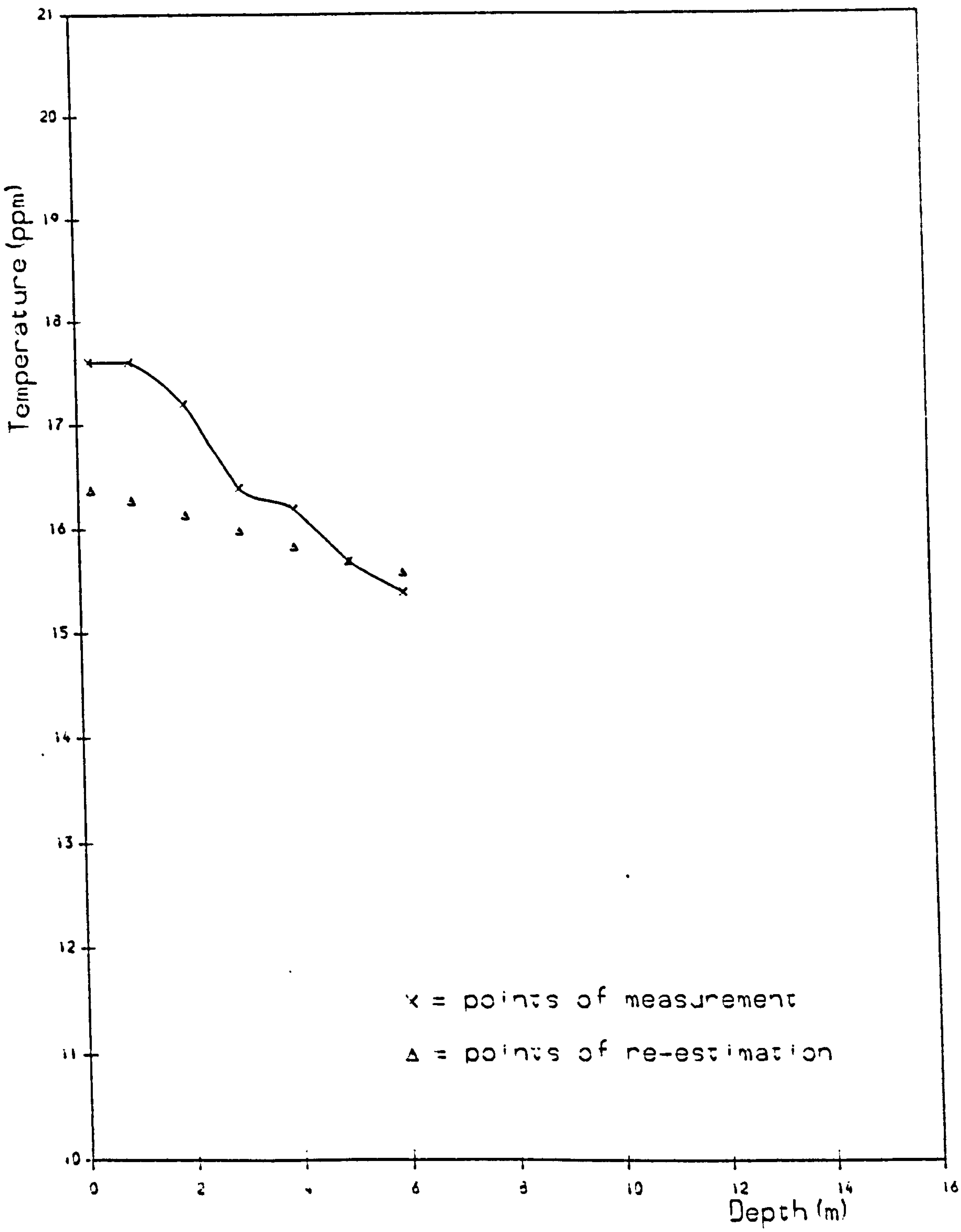

Fig. 4.13 Comparison between measurements and re-estimations

station 7 High Water

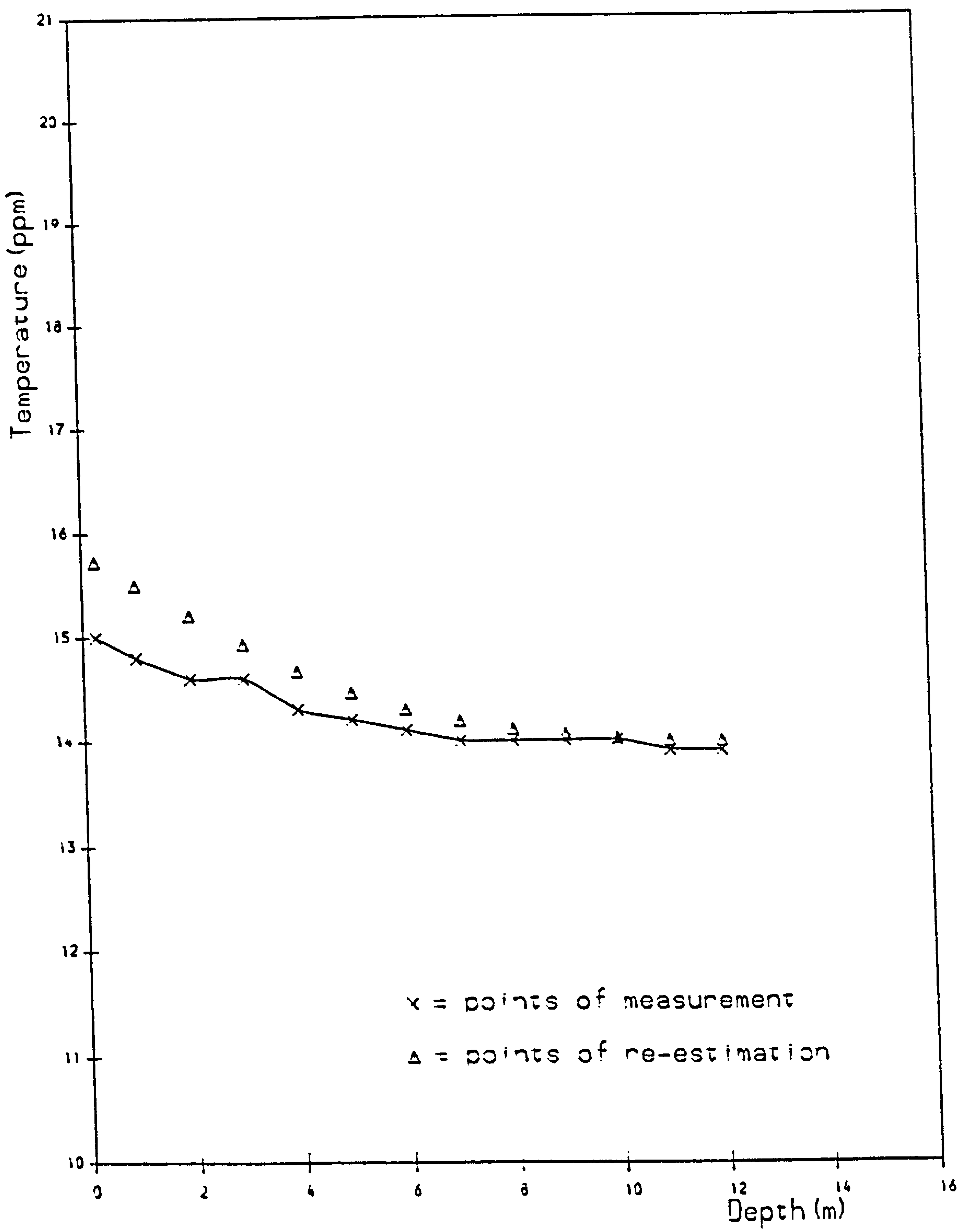

Fig. 4.14 Comparison between measurements and re-estimations

station 5 High Water

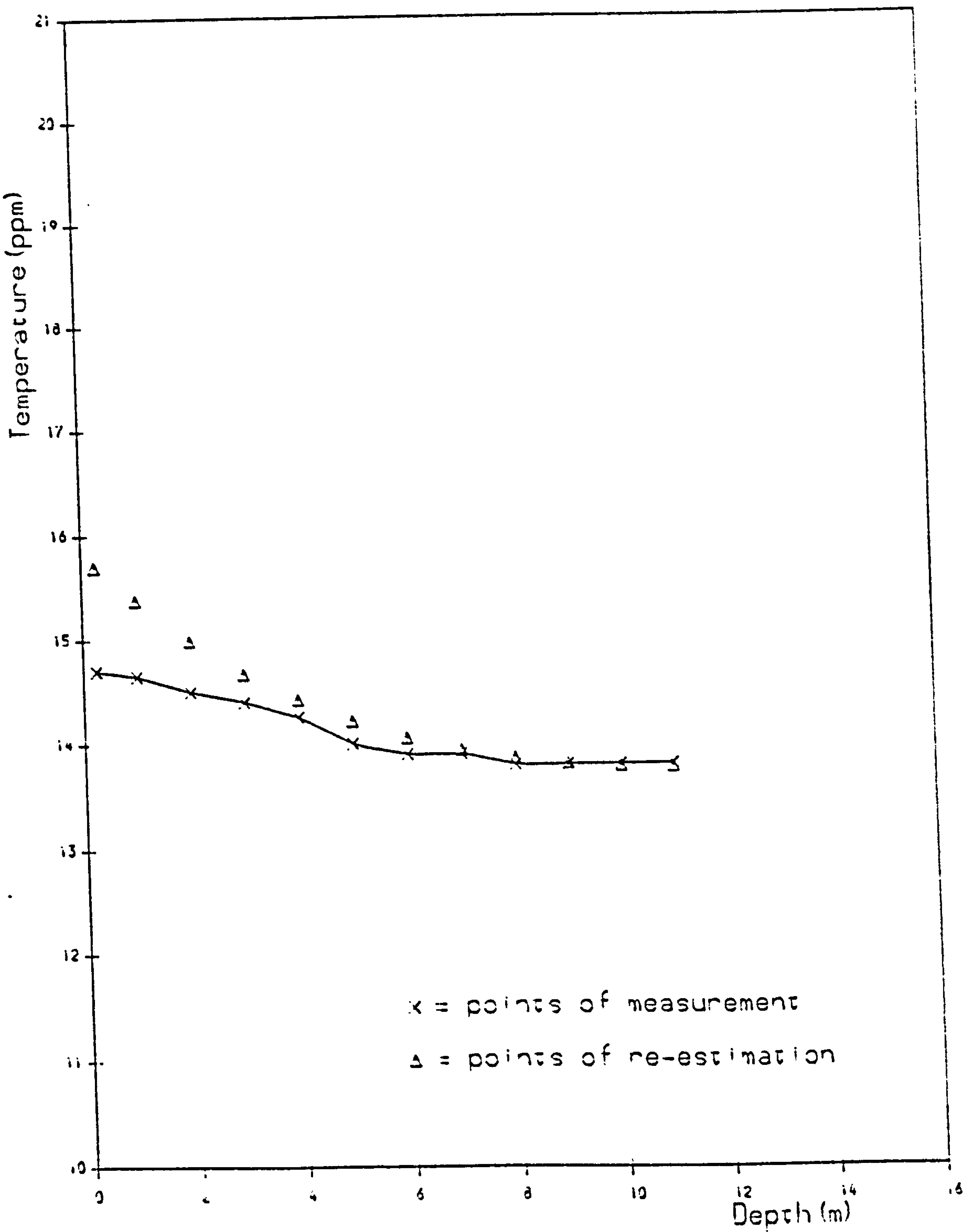

Fig. 4.15 Comparison between measurements and re-estimations

station 4 High Water

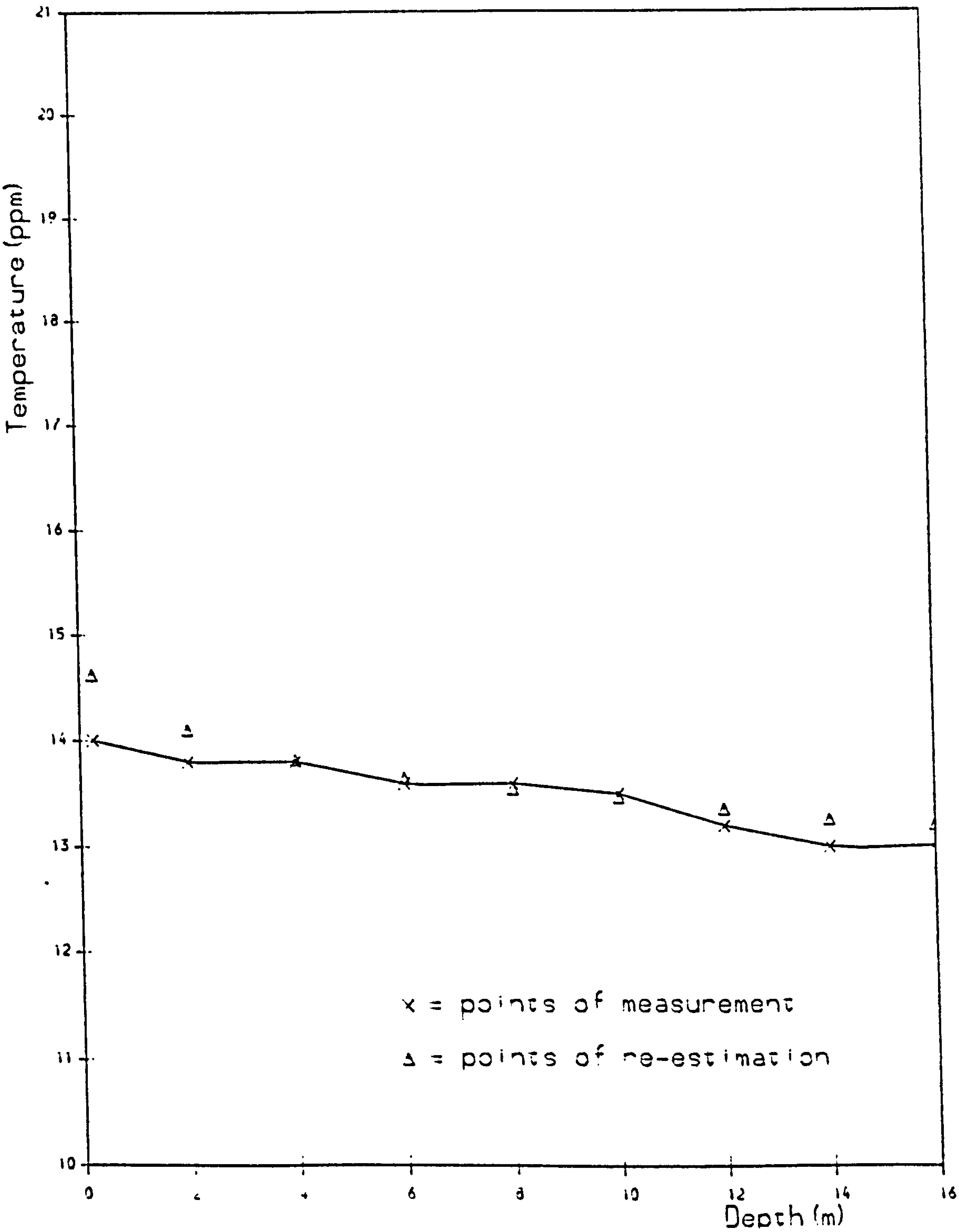

Fig. 4.16 Comparison between measurements and re-estimations

station 2 High Water

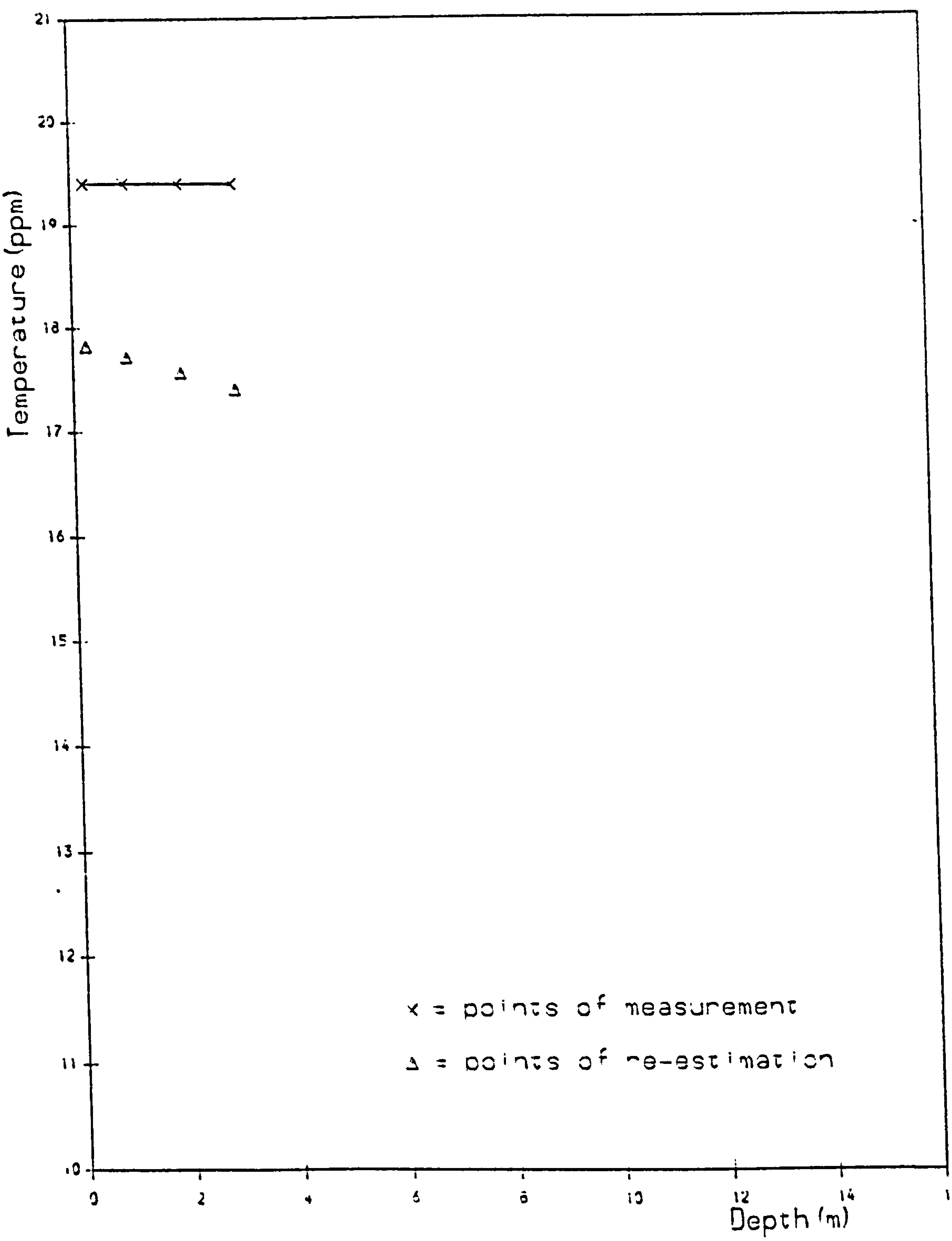

Fig. 4.17 Comparison between measurements and re-estimations
station 7 Mid Tide

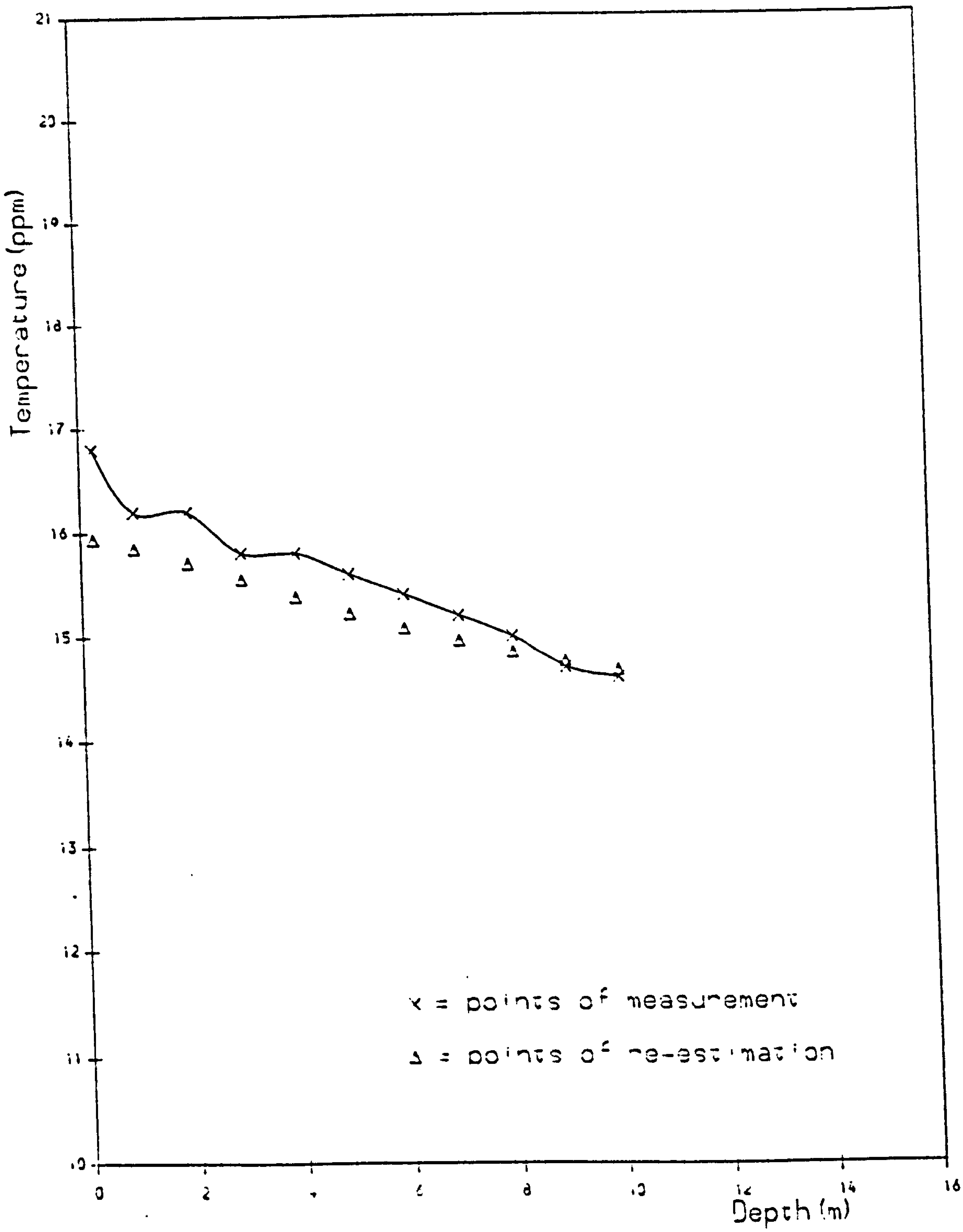

Fig. 4.18 Comparison between measurements and re-estimations
station 5 Mid Tide

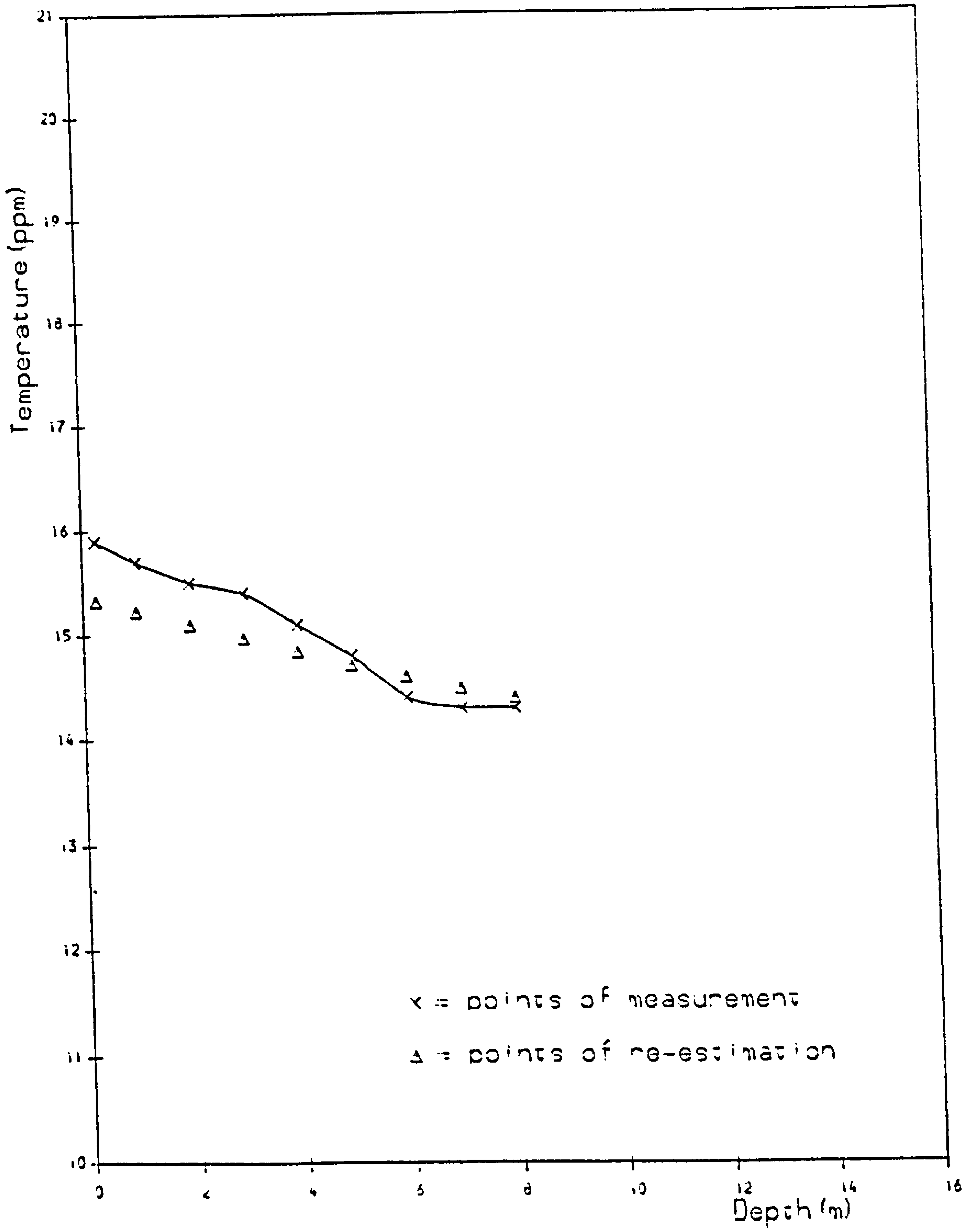

Fig. 4.19 Comparison between measurements and re-estimations
station 4 Mid Tide

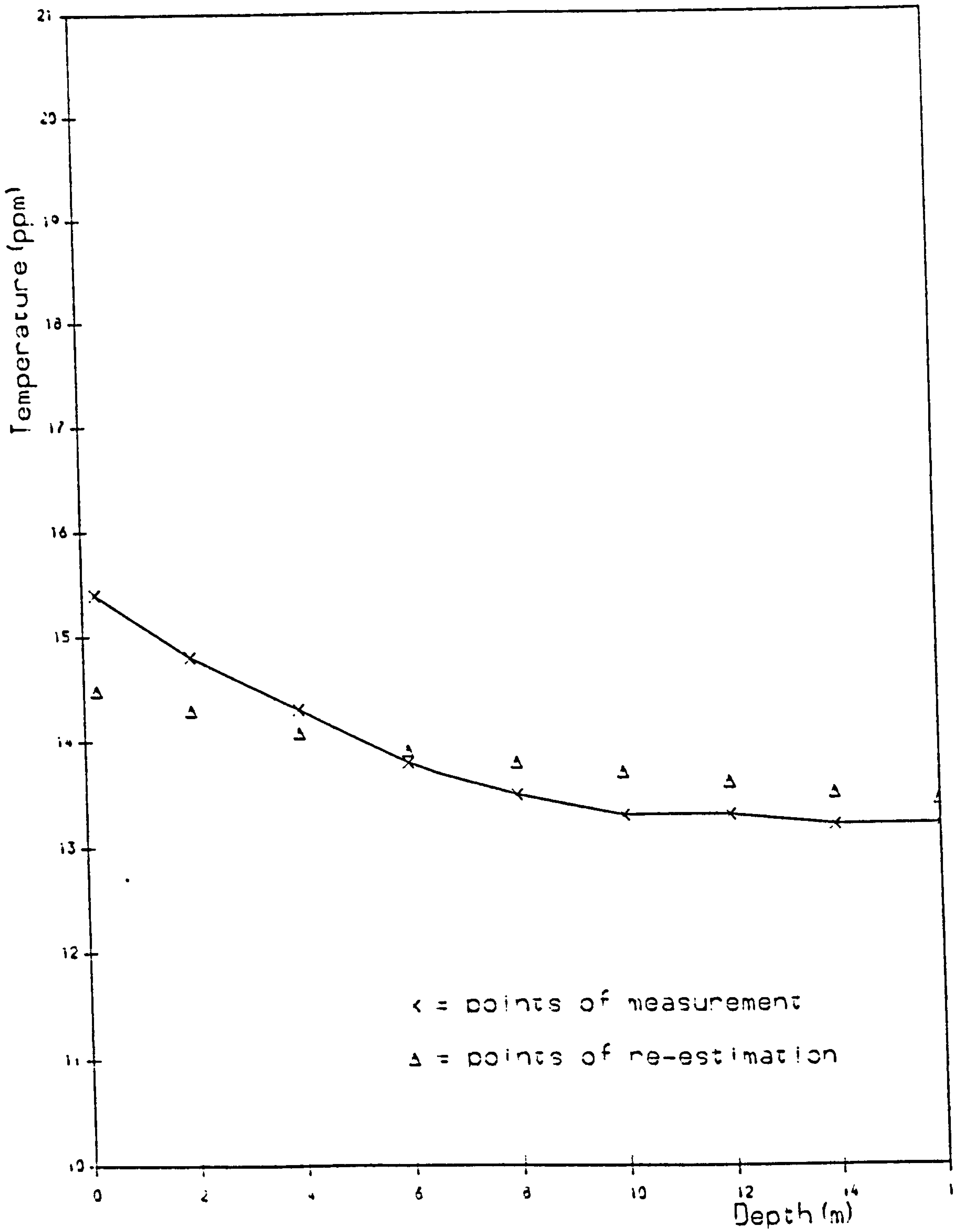

Fig. 4.20 Comparison between measurements and re-estimations
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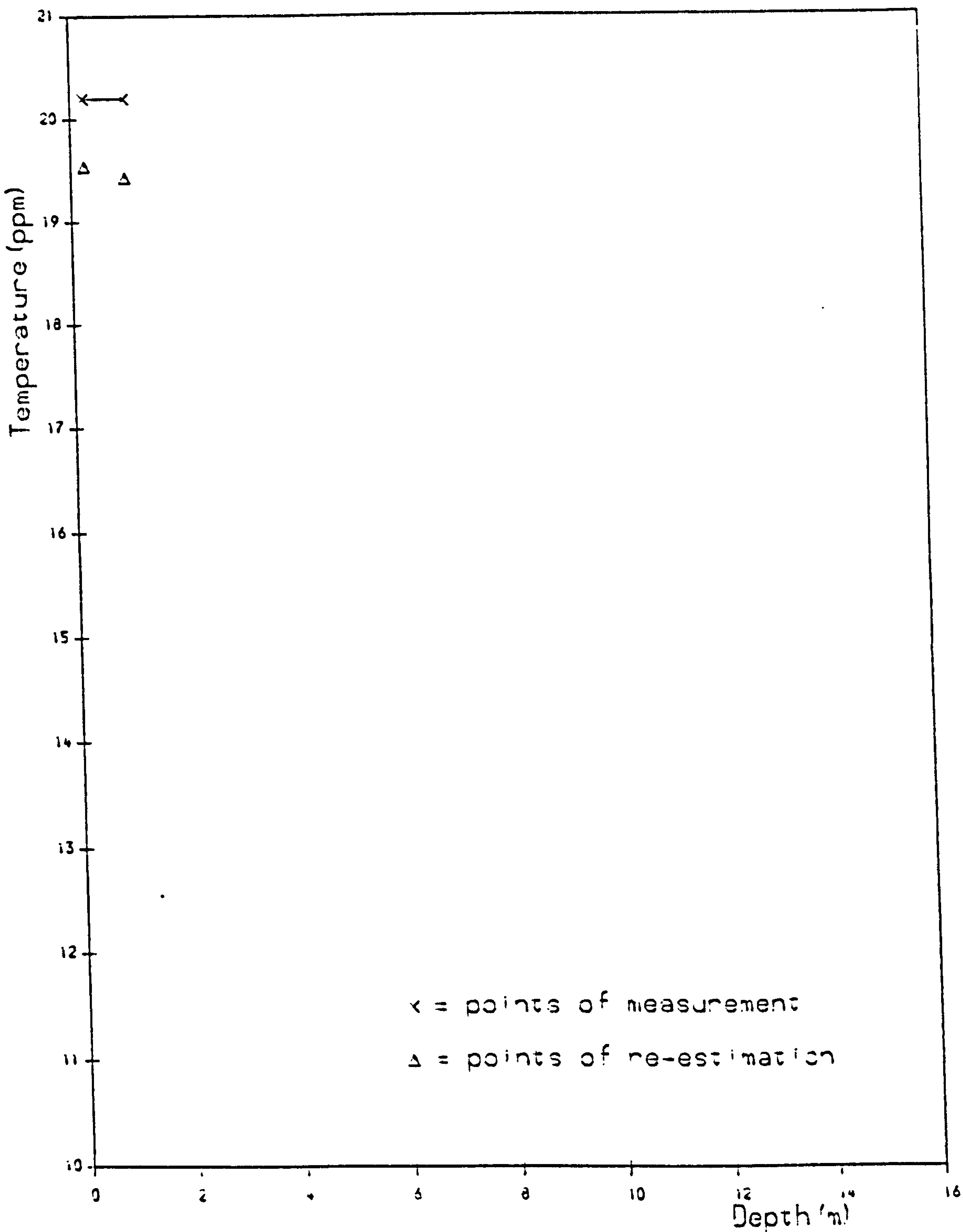


Fig. 4.21 Comparison between measurements and re-estimations

station 7 Low Water

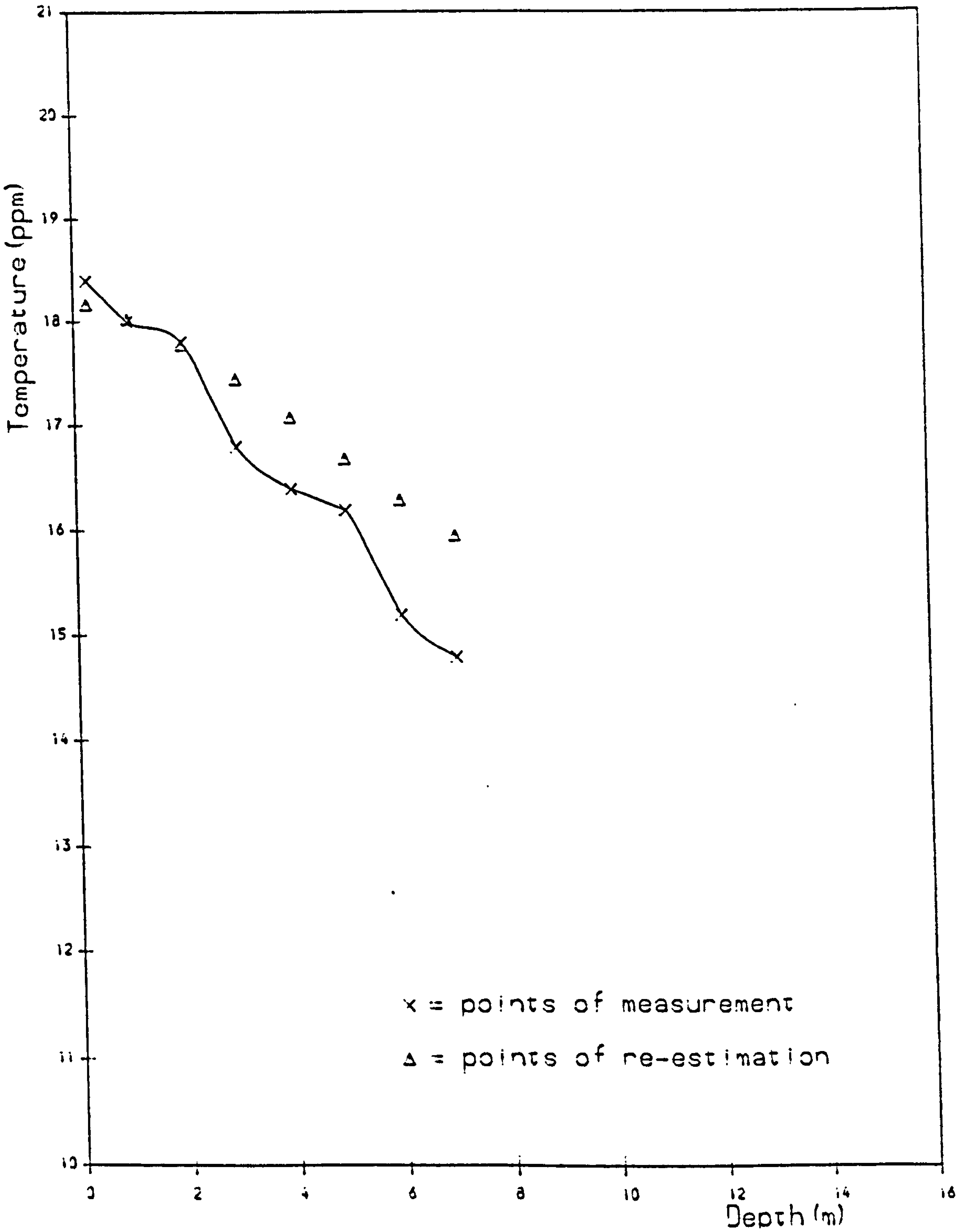


Fig. 4.22 Comparison between measurements and re-estimations

station 5 Low Water

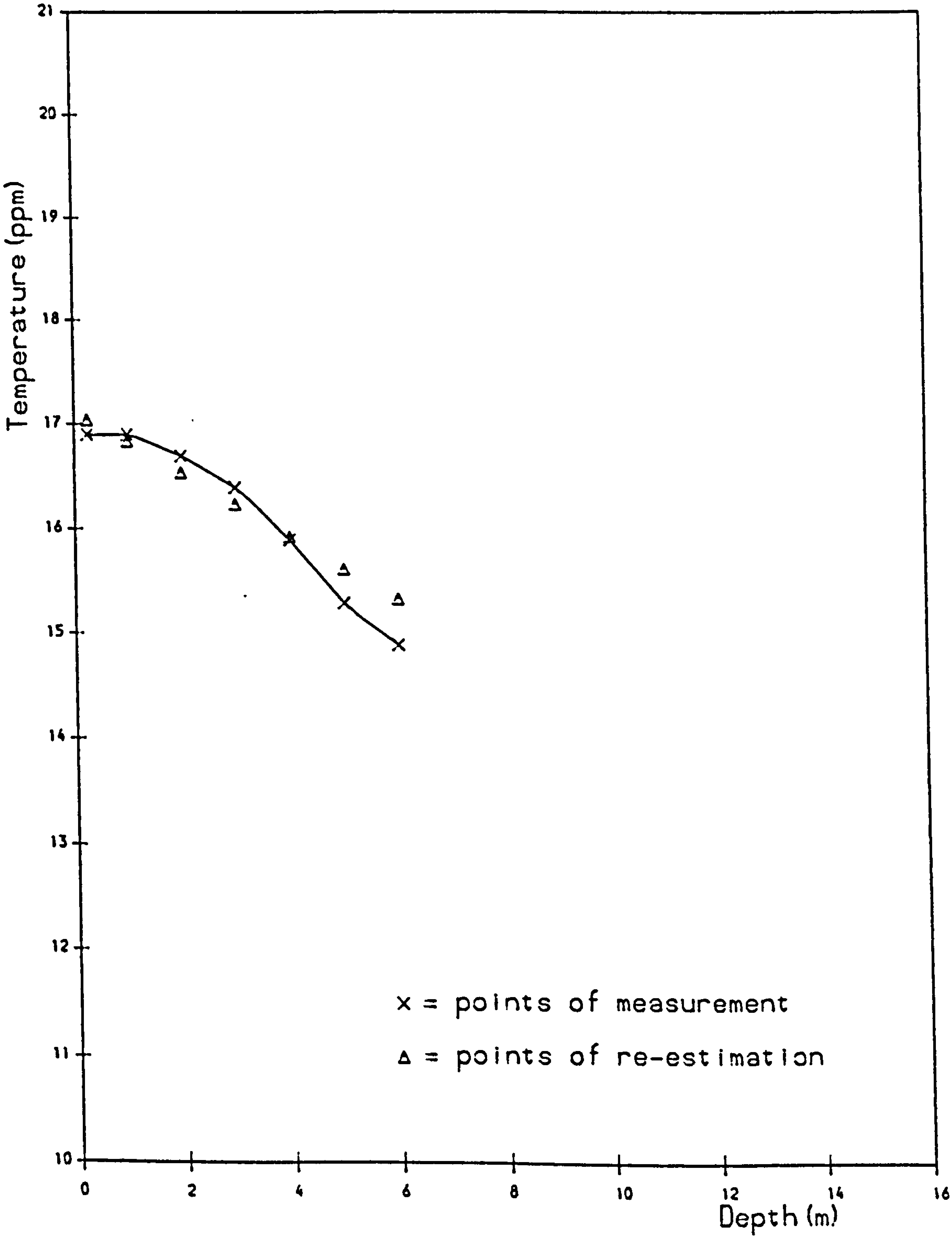


Fig. 4.23 Comparison between measurements and re-estimations

station 4 Low Water

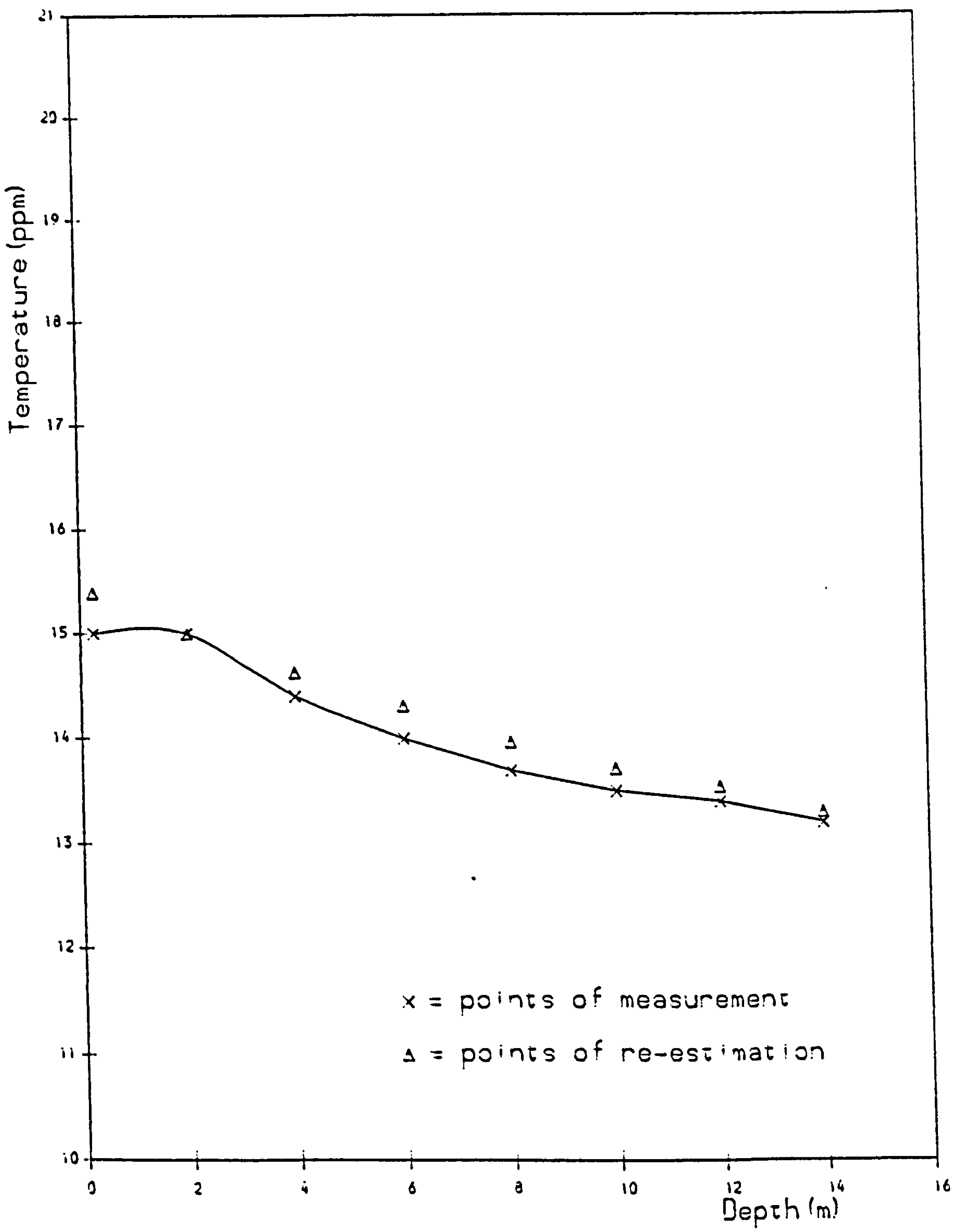


Fig. 4.24 Comparison between measurements and re-estimations

station 2 Low Water

Chapter 5 Introduction to Numerical Methods

5.1 Introduction

Many problems in the physical sciences and engineering are posed mathematically in terms of equations involving derivatives of the function which expresses the relationship one seeks. Such an equation is called a *differential equation.* There are two classes of differential equations: ordinary differential equations and partial differential equations. An ordinary differential equation only involves derivatives of one variable, while, a partial differential equation involves one or more partial derivatives of two or more independent variables. The problem then is how to solve the differential equation. The best way to solve any physical problems governed by a differential equation is to obtain the analytical solution. However, there are many situations where the analytical solution is difficult to obtain, and the only recourse is to use some technique for approximating the numerical values of the solution. Because of the development of fast computers and effective softwares, many problems previously beyond one's capability can now be solved approximately to a high degree of accuracy.

A numerical method can be used to obtain an approximate solution for the above purpose. All numerical solutions produce values at discrete points within the domain of required solution. Numerical solutions are more desirable than no solution at all because the calculated values provide important information about the physical process.

There are several procedures for obtaining a numerical solution of a differential equation. The corresponding methods can be classified into four categories:(1) the finite difference method, (2) the variational method, (3) the weighted residuals method, and (4) the finite element method. The following sections will describe those methods separately.

5.2 The Finite Difference Method

The finite difference method has a long history and a well-established literature. Here, only is a brief description of the method to be introduced. A systematic description of the method can be found in the books by authors(Smith, 1985; Peaceman, 1977)

The numerical solution of differential equations by finite difference refers to the process of approximating the derivatives by finite difference quotients, and then obtaining solutions of the resulting system of the algebraic equations. Consider a function of three independent variables u(x,y,t), a first derivative can be approximated in three ways:

(1) a forward-difference quotient:

$$\frac{\partial u(x,y,t)}{\partial x} \simeq \frac{u(x+\Delta x,y,t)-u(x,y,t)}{\Delta x} \qquad 5.1$$

(2) a backward-difference quotient:

$$\frac{\partial u(x,y,t)}{\partial x} \simeq \frac{u(x,y,t)-u(x-\Delta x,y,t)}{\Delta x} \qquad 5.2$$

(3) a centered-difference quotient:

$$\frac{\partial u(x,y,t)}{\partial x} \simeq \frac{u(x+\Delta x,y,t)-u(x-\Delta x,y,t)}{2\Delta x} \qquad 5.3$$

and a second derivative can be approximated by a centered second-difference quotient:

$$\frac{\partial^2 u(x,y,t)}{\partial x^2} \simeq \frac{u(x+\Delta x,y,t)-2u(x,y,t)+u(x-\Delta x,y,t)}{\Delta x^2} \qquad 5.4$$

Other derivatives $\frac{\partial u}{\partial y}$, $\frac{\partial^2 u}{\partial y^2}$, $\frac{\partial u}{\partial t}$ etc. can be derived in the forms like the above ones.

The accuracy of each difference-quotient may be obtained by using the Taylor series expansions. The difference-quotients (5.1) and (5.2) are of first-order accuracy, while (5.3) and (5.4) are of second-order accuracy.

Fundamental to both the finite element and finite difference approaches of solving differential equations is the concept of discretization. Discretization means that the solution domain is divided by a set of grids. There are two types of grids commonly used in the finite difference method. Either a block-centered or point-centered grid can be employed. They are illustrated in Fig. 5.1

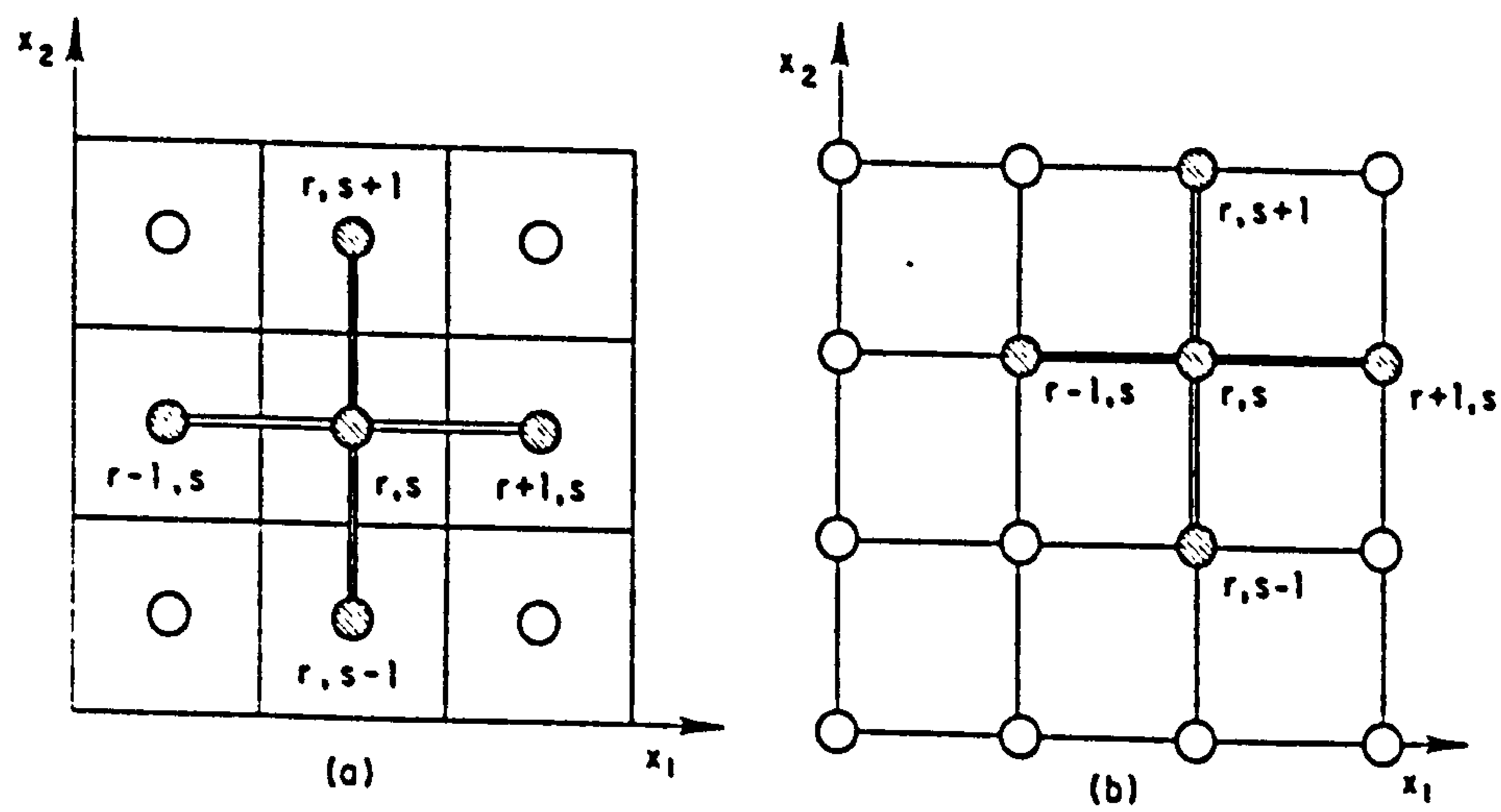


Fig. 5.1 Block-centered (a) and mesh-centered(b) finite difference approximations (After Huyakorn, 1983)

The finite difference equations are written in the same way for either grid system. However, it should be pointed out that the treatment at boundaries of the solution domain is quite quite different in the two cases of grid systems.

A numerical solution of a finite difference equation must be stable and convergent. Stability refers to the behavior of round-off errors encountered during algebraic manipulations. A numerical solution will be considered stable if such an error is damped with time. Convergence, on the other hand, considers the behavior of truncation error due to the replacement of a derivative by difference quotient. Convergence of a numerical solution is achieved when the error in the solution tends to zero uniformly with mesh refinement, i.e., as $\Delta x \rightarrow 0 (or \Delta y \rightarrow 0, \Delta z \rightarrow 0)$ and $\Delta t \rightarrow 0$. It can be shown that stability is both a necessary and sufficient condition for convergence if certain supplementary conditions are fullfilled.

5.3 The Variational Method

In this method, a functional is formulated from the differential equations. A solution of the differential equations makes the functional minimum. Also, a function of the state variable which makes the functional minimum must be a solution of the differential equations. Given the differential equations, an approximate solution can be obtained by substituting different trial functions into the approximate functional. The trial function that gives the minimum value of the functional is the approximate solution.

The crux of the method is how to construct a functional for a given differential equation. Generally, there are two ways to formulate a functional. First, the relevant functional can be found directly from familiar physical principles. For example, the expression of the total potential energy in structural and elastic continum problems is a functional equivalent to the differential equation of the problem. Second, the functional forms are already known for certain types of differential equations, details can be found in the book by Karadestunoer(1987). It should be noted that there does not always exist a functional for each different problem.

After the establishment of the functional, the unknown function minimizing the functional must be obtained to get a solution the problem. Suppose the analysis of a physical or engineering problem using the differential equation as

$$L[\phi] = f \qquad 5.5$$

where L is a differential operator, ϕ is the state variable to be calculated, and f is a given function of position. In addition, ϕ must satisfy the boundary conditions:

$$B_i[\phi] = q_i|_{at\ boundary\ c_i} \qquad i = 1, 2, \ldots \qquad 5.6$$

Let Π be the functional of the variational problem that is equivalent to the the differential formulation given in (5.5) and (5.6). The Rayleigh-Ritz method provides an algorithm for minimizing a given functional. The basic step in the Rayleigh-Ritz method is to assume a solution of the form

$$\tilde{\phi} = \sum_{i=1}^{n} a_i \psi_i \qquad 5.7$$

where the ψ_i are linearly independent trial functions and the a_i are multiplies to be determined in the solution.

In the Rayleigh-Ritz method, the trial function $\tilde{\psi}$ given as (5.7) is substituted into Π, and n simultaneous equations for the parameters a_i are generated using the minimum condition of Π

$$\frac{\partial \Pi}{\partial a_i} = 0 \quad , \qquad i = 1, 2, \ldots, n \tag{5.8}$$

which results in a set of n algebraic equations in n unknown $a_1, a_2, \ldots, a_n$.

As mentioned before, there may not exist an appropriate functional corresponding to a given problem. In this case, the Rayleigh-Ritz method is not applicable. Thus, a more general method should be sought. The next section will introduce such a method.

5.4 The Method of Weighted Residuals

This method also involves an integral like the one in the variational method, but the fundamental difference between the two methods is that the weighted residual method operates directly on the differential equations of a given problem while the variational method operates on its equivalent variational principle.

As usual, consider the boundary value problem shown by (5.5) and (5.6)

$$L[\phi] = f \qquad in\ R$$

$$B_i[\phi] = q_i|_{at\ boundary\ c_i} \qquad i = 1, 2, \ldots$$

The weighted residual method starts with an approximate solution $\tilde{\phi}$ defined by (5.7)

$$\tilde{\phi} = \sum_{i=1}^{n} a_i \psi_i$$

Then, the approximate solution is substituted into the differential equations. Since the approximate solution $\tilde{\phi}$ will not , in general, satisfy the equations, a residual or error term results as defined by

$$r(\tilde{\phi}) = L(\tilde{\phi}) - f = L[\sum_{i=1}^{n} a_i \psi_i] - f$$

For the exact solution ϕ_o, then

$$r(\phi_o) = 0$$

The essential idea of the weighted residual method is that the unknown parameters $\{a_i\}$ are determined so as to make the weighted average of $r(\tilde{\phi})$ vanish. There are several criteria to make a weighted average of $r(\tilde{\phi})$ zero. These methods are described as follows.

Collocation Method: in this method the residual $r(\tilde{\phi})$is set equal to zero at n distinct points in the solution domain to obtain n simultaneous equations for the set of unknown parameters a_i.

Subdomain Method: in this method the complete domain of solution is subdivided into n subdomains, and the integral of the residual over each subdomain is set equal zero to generate n equations for the parameters a_i.

Least Square Method: in this method the integral of the square of the residual is minimized with respect to the parameter a_i

$$\frac{\partial}{\partial a_i}\int_D r^2(\tilde{\phi})\, dD = 0 \quad , \qquad i = 1, 2, \ldots, n$$

Galerkin Method: in this method the parameters a_i are determined from the n equations

$$\int_D \psi_i r \, dD = 0 \quad , \qquad i = 1, 2, \ldots, n$$

where D is the solution domain.

The four methods seem different from each other, but all of them can be derived from a unified form

$$\int_D W_i r(\tilde{\phi})\, dD = 0$$

where W_i is a weighting function, in cases of

(1) Collocation Method: $W_i = \delta_i$, δ_i: impulse function

(2) Subdomain Method: $W_i = 1$ over each subdomain

(3) Least Square Method: $W_i = r(\tilde{\phi})$ the residual as the weighting function

(4) Galerkin Method: $W_i = \psi_i$ the basis function as the weighting function

So far, the boundary conditions have not yet been discussed in those methods. There are two classes of boundary conditions called essential and natural boundary conditions. The essential boundary conditions are also called *geometric boundary conditions*; namely, they correspond to prescribed values of the solution function. The natural boundary conditions are also called *forced boundary conditions*; namely, the natural boundary conditions correspond to prescribed derivatives of the solution function. It is useful to distinguish the two classes of boundary conditions because they need be treated differently.

In weighted residual methods, boundary conditions can be treated in two ways. Firstly, the basis functions ψ_i in (5.5) are chosen so as to satisfy all essential and natural boundary conditions. Thus, only trial functions that satisfy all boundary conditions can be employed. Secondly, the basis functions ψ_i in (5.5) are chosen so as to only satisfy essential boundary conditions, while the natural boundary conditions are satisfied by including them in the formulation of the weighted residual method.

In contrast, these functions ψ_i in the Rayleigh-Ritz analysis need only satisfy the essential boundary condition because the functional in a variational formulation implicitly contains the natural boundary conditions. Hence, for approximate solutions, a larger class of trial functions can be employed. This is one apparent advantage of using the variational method.

Although the basis function ψ_i in the weighted residual method need not satisfy conditions, the Rayleigh-Ritz method still possesses some significant advantages over the weighted residual method. First, the Rayleigh-Ritz method requires less continuity in the solution function, i.e., the function employed in the weighted residual method must be as twice differentiable as the ones employed in the Rayleigh-Ritz method. Second, the Rayleigh-Ritz method always yields a symmetric coefficient matrix, whereas the weighted residual method results in a nonsymmetric one which is less efficient computationally.

The variational method possesses the above two advantages, but it is only applicable when a suitable functional exists. Meanwhile, the weighted residual method can be applied to any differential equations which may have a corresponding functional or not. This is an apparent advantage of the weighted residual method over the variational method. What is more, the Galerkin method can yield the same results as the variational method when applied to self-adjoint differential equations.

5.5 The Finite Element Method

The finite element method is a numerical method for solving differential equations by means of "piecewise approximation". It originated in the field of structural analysis and was widely developed and exploited in other fields such as aeronautical engineering, water resources etc.. More applications of the method can be found in the books by authors Zienkiewicz(1979), Bath(1982), Pinder(1975) ...

To know what the finite element method is, it is important to understand the concept of finite elements. In the finite element method , the solution domain is divided into subdomains which are called finite elements. Such elements may take triangular, quadrilateral shapes in case of two dimensional domain. The basis functions adopted usually are polynomials which are piecewise continuous over finite elements. Nodes are located along the boundaries of each finite element and each basis function is defined at a specific node. On the base of finite element concept, previous methods , i.e., variational method and weighted residual method, are applied to each element instead of the entire domain. Thus, different finite element methods can be formed with combinations of different methods. For example, there are the Galerkin-finite element method, collocation-finite element method, and the Rayleigh-Ritz finite element method.

The various steps involved in the solution of any problems by a finite element method may be summarised as follows:

1. Discretize the region of solution into a finite number of subdomains, the finite elements. Such elements can be line intervals in one dimension domain, triangles and quadrilaterales in two dimension domain, and tetrahedra and rectangular bricks in three dimension domain. Each element is numbered by its element and node numbers , and is located by its nodal coordinate values. Finer elements should be placed to the region where the solution changes abruptly.

2. Choose nodal variables and shape functions. In most problems, unknown nodal values of the solution are used as the variables, and polynomials are usually used as shape functions with different orders.

3. Develope an element matrix for each element. The element matrix can be established by either the variational method or the weighted residual method.

4. Assemble the overall matrix over the solution domain from the individual element matrices.

5. Incooperate the essential boundary conditions into the global matrix.

6. Solve the global matrix. There are different solution methods available, for example, the Gauss elimination method.

These six steps are used in the next chapter during the formulation of the Galerkin-finite element method. More details are illustrated and discussed there.

Before finishing this chapter, some comparisons among all the numerical methods described so far are necessary. First, the finite element is compared with the finite difference method. In the finite element method the nodal values are simply parameters associated with a piecewise polynomial function defined throughout the solution domain. In the finite difference solution the nodal points are only points at which the solution is defined. In other words, any unknown solution values can be obtained through the trial function in the finite element method, but can only be obtained through interpolation in the finite difference method. Second, the finite element method is compared with the weighted residual method. In the finite element method, the trial function is fit to each element and the whole trial function is the sum of trial functions from each element. In the weighted residual method the trial function is fit to the whole solution domain, i.e., the whole domain is treated equally.

Up to now, a basic knowledge of numerical methods has been briefly illustrated. It could be applied to practical problems for one's need. The next chapter is such a topic.

Chapter 6 Formulation of Water Quality Models

6.1 Introduction

Water is one of the materials that are indispensable to the existence of human beings. At present, water quantity is not a primary concern to many people, but water quality has been emerging as a serious problem threatening our environment, due to the pollution caused by two main waste sources. First, as modern population has been increasing dramatically, a large amount of domestic waste has resulted. Second, as modern industries have been developing rapidly, an even larger amount of industrial waste has been produced.

It has long been known that all natural bodies of water have the ability to oxidize organic matters without the development of nuisance condition, provided that the organic loading is kept within the limit of the oxygen resources of the water. Hence, natural bodies of water , such as rivers and estuaries, have been taken for granted as ideal dumping sites for the disposal of domestic and industrial wastes. Subsequently, many of them have been polluted to a different degree because of receiving too many waste loads without the regard of their capacity for dilution and purification of wastes. Clearly, the concentration of Dissolved Oxygen (DO) in water is a good indication of the water quality, and the pollution strength of wastes can be defined in terms of Biochemical Oxygen Demand (BOD) which is usually defined as the amount of oxygen required by bacteria while stabilizing decomposable organic matter under aerobic conditions.

In order to control and predict water quality, it is essential to be able to know the variation of DO in space and time under a certain BOD load. Thus, a model should be employed to find the BOD/DO relationship. The model classes may be defined: (1) analytical models like the Streeter-Phelps model, (2) hydraulic models(McDowell, 1977; Ward, 1971), and (3) numerical models(Ward, 1971). Only numerical models are considered as possessing the capability to simulate complicated situations. Therefore, numerical models were chosen to be developed in this chapter. A numerical model is the product of a numerical method applied to a practical problem. In chapter 5, commonly used numerical methods were described. In this chapter, first the problem is presented as a set of governing equations, and then a detailed model formulation of finite element method is given, last the structure of the program of the finite element model is outlined.

6.2 Governing Equations

As the basis for prediction of water quality, it is necessary to derive the basic time-dependent equations in three spatial dimensions, expressing the conservation of mass and momentum in estuaries. Many books (Ward, 1971; Park, 1985) contain a very detailed derivation of these equations, therefore, only a brief description of the governing equations are presented next.

The basic statement of the principle of conservation of mass is that the change in mass over a time interval δt for a fixed volume of fluid is equal to the difference between the inflow to and the outflow from the volume over the same time interval δt. Thus, this statement leads to the differential equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0 \qquad 6.1$$

$$\frac{\partial c}{\partial t}+\frac{\partial cu}{\partial x}+\frac{\partial cv}{\partial y}+\frac{\partial cw}{\partial z}=0 \qquad 6.2$$

where

ρ = the fluid density

c = the concentration of diffusing conservative solutes

u, v, w = the components of fluid velocity in the X,Y,Z direction

The equation 6.1 may be expanded to the form

$$\frac{\partial \rho}{\partial t}+u\frac{\partial \rho}{\partial x}+v\frac{\partial \rho}{\partial y}+w\frac{\partial \rho}{\partial z}+\rho(\frac{\partial u}{\partial t}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z})=0 \qquad 6.3$$

In equations 6.1 and 6.2 the mass transport by the molecular diffusion is neglected. Equation 6.1 is the general statement of the continuity equation for any fluid compressible or incompressible. In mathematical terms, the first four terms of equation 6.3 relates the change in density of an individual particle as it moves through time and space, and may be written as

$$\frac{d\rho}{dt}=\frac{\partial \rho}{\partial t}+u\frac{\partial \rho}{\partial x}+v\frac{\partial \rho}{\partial y}+w\frac{\partial \rho}{\partial z}$$

Equation 6.3 then can be written as

$$\frac{d\rho}{dt}+\rho(\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z})=0 \qquad 6.4$$

If a fluid is incompressible, as may be taken the case for the water in estuaries under most circumstances, then

$$\frac{d\rho}{dt} = 0$$

and the equation 6.4 become

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \qquad 6.5$$

which is the volumetric continuity equation for an incompressible fluid.

The basic statement of the principle of momentum is that the time rate of change of momentum of a moving elemental fluid is equal to the sum of the forces acting on the particle, that is, Newton's Second Law of Motion. Thus, the differential equation expressing this principle is formulated as

$$\frac{d\mathbf{V}}{dt} = -\frac{1}{\rho}\nabla P + \mathbf{f} \bullet \mathbf{V} + \mathbf{g} + \mu(\nabla^2 \mathbf{V}) \qquad 6.6$$

The above equation may be expanded as

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + fv + \mu(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}) \qquad 6.7$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + w\frac{\partial v}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial y} + fu + \mu(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}) \qquad 6.8$$

$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}=-\frac{1}{\rho}\frac{\partial p}{\partial z}-g+\mu(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}) \quad 6.9$$

where

x,y,z = Cartesian coordinates, positive eastward, northward, and upward respectively

u,v,w = respective components of velocity

t = time

f = $2\Omega sin\psi$, Coriolis parameter, Ω the angular velocity of the earth, ψ the latitude

P = pressure

ρ = density

μ = the kinematic molecular viscosity

g = the acceleration of gravity

Usually, equation 6.9 may be reduced to the hydrostatic equation by neglecting the vertical acceleration terms of velocity compared to the gravity in the vertical component. Thus, equation 6.9 is rewritten as

$$0=-\frac{1}{\rho}\frac{\partial P}{\partial z}-g \quad 6.10$$

All the above equations are valid only at instant time scale. In practice, the instantaneous values of the state variables concerned like velocity are difficult to measure due to the fast random fluctuation caused by turbulence, and only time averaged velocities are measured. The relationship between an instantaneous value and a time averaged value can be linked by a fluctuation component, and can be expressed as

$$u = \widetilde{u} + u' \tag{6.11}$$

$$v = \widetilde{v} + v' \tag{6.12}$$

$$w = \widetilde{w} + w' \tag{6.13}$$

$$P = \widetilde{P} + P' \tag{6.14}$$

$$\rho = \widetilde{\rho} + \rho' \tag{6.15}$$

$$c = \widetilde{c} + c' \tag{6.16}$$

where

u,v,w = the instantaneous velocity components in the X, Y, Z directions respectively

P = the instantaneous value of pressure

ρ = the instantaneous value of density

c = the instantaneous concentration of diffusing solutes

$\tilde{u}, \tilde{v}, \tilde{w}$ = the mean velocity in the X, Y, Z directions over time interval Δt

$\tilde{P}$ = the mean pressure over the time interval Δt

$\tilde{\rho}$ = the mean density over the time interval Δt

$\tilde{c}$ = the mean concentration over the time interval Δt

u', v', w' = the velocity fluctuations with respect to the mean values in the X, Y, Z directions

P' = the fluctuation in pressure

ρ' = the fluctuation in density

c' = the fluctuation in concentration

the mean value and fluctuation are defined as

for example

$$\tilde{u} = \frac{1}{\Delta t} \int_0^{\Delta t} u dt$$

$$\tilde{u}' = \frac{1}{\Delta t} \int_0^{\Delta t} u' dt = 0$$

By substituting equations (6.11 - 6.16) into all previous equations and averaging them over time interval Δt, the continuity equation 6.5 become

$$\frac{\partial\tilde{u}}{\partial x}+\frac{\partial\tilde{v}}{\partial y}+\frac{\partial\tilde{w}}{\partial z}=0 \qquad 6.17$$

the momentum equations (6.6 - 6.9) become

$$\begin{aligned}\frac{\partial\tilde{u}}{\partial t}+\tilde{u}\frac{\partial\tilde{u}}{\partial x}+\tilde{v}\frac{\partial\tilde{u}}{\partial y}+\tilde{w}\frac{\partial\tilde{u}}{\partial z} &= -\frac{1}{\tilde{\rho}}\frac{\partial\tilde{P}}{\partial x}+f\tilde{v}+\mu\left(\frac{\partial^2\tilde{u}}{\partial x^2}+\frac{\partial^2\tilde{u}}{\partial y^2}+\frac{\partial^2\tilde{u}}{\partial z^2}\right)\\ &\quad -\left(\frac{\partial\widetilde{u'u'}}{\partial x}+\frac{\partial\widetilde{u'v'}}{\partial y}+\frac{\partial\widetilde{u'w'}}{\partial z}\right)\end{aligned} \qquad 6.18$$

$$\begin{aligned}\frac{\partial\tilde{v}}{\partial t}+\tilde{u}\frac{\partial\tilde{v}}{\partial x}+\tilde{v}\frac{\partial\tilde{v}}{\partial y}+\tilde{w}\frac{\partial\tilde{v}}{\partial z} &= -\frac{1}{\tilde{\rho}}\frac{\partial\tilde{P}}{\partial y}+f\tilde{u}+\mu\left(\frac{\partial^2\tilde{v}}{\partial x^2}+\frac{\partial^2\tilde{v}}{\partial y^2}+\frac{\partial^2\tilde{v}}{\partial z^2}\right)\\ &\quad -\left(\frac{\partial\widetilde{v'u'}}{\partial x}+\frac{\partial\widetilde{v'v'}}{\partial y}+\frac{\partial\widetilde{v'w'}}{\partial z}\right)\end{aligned} \qquad 6.19$$

$$\begin{aligned}\frac{\partial\tilde{w}}{\partial t}+\tilde{u}\frac{\partial\tilde{w}}{\partial x}+\tilde{v}\frac{\partial\tilde{w}}{\partial y}+\tilde{w}\frac{\partial\tilde{w}}{\partial z} &= -\frac{1}{\tilde{\rho}}\frac{\partial\tilde{P}}{\partial z}-g+\mu\left(\frac{\partial^2\tilde{w}}{\partial x^2}+\frac{\partial^2\tilde{w}}{\partial y^2}+\frac{\partial^2\tilde{w}}{\partial z^2}\right)\\ &\quad -\left(\frac{\partial\widetilde{w'u'}}{\partial x}+\frac{\partial\widetilde{w'v'}}{\partial y}+\frac{\partial\widetilde{w'w'}}{\partial z}\right)\end{aligned} \qquad 6.20$$

Equations (6.17 - 6.20) are usually called Reynold's Equations because the additional terms like $\widetilde{u'u'}, \widetilde{u'v'}$ etc. may be approximated by applying the concept of Reynold's stress.

Equation 6.2 become

$$\frac{\partial\tilde{c}}{\partial t}+\frac{\partial}{\partial x}(\tilde{u}\tilde{c})+\frac{\partial}{\partial y}(\tilde{v}\tilde{c})+\frac{\partial}{\partial z}(\tilde{w}\tilde{c})+\frac{\partial}{\partial x}(\widetilde{u'c'})+\frac{\partial}{\partial y}(\widetilde{v'c'})+\frac{\partial}{\partial z}(\widetilde{w'c'})=0 \qquad 6.21$$

in which the last three terms are approximated by the analogy with the Fick's Law as

$$\widetilde{u'c'} = -D_x \frac{\partial \tilde{c}}{\partial x}$$

$$\widetilde{v'c'} = -D_y \frac{\partial \tilde{c}}{\partial y}$$

$$\widetilde{w'c'} = -D_z \frac{\partial \tilde{c}}{\partial z}$$

where D_x, D_y, D_z = turbulent diffusion coefficients in X, Y, Z directions respectively

With these substitutions, Equation (6.21) becomes the so-called three dimensional convection - diffusion equation

$$\frac{\partial \tilde{c}}{\partial t}+\frac{\partial}{\partial x}(\tilde{u}\tilde{c})+\frac{\partial}{\partial y}(\tilde{v}\tilde{c})+\frac{\partial}{\partial z}(\tilde{w}\tilde{c})-\frac{\partial}{\partial x}(D_x\frac{\partial \tilde{c}}{\partial x})-\frac{\partial}{\partial y}(D_y\frac{\partial \tilde{c}}{\partial y})-\frac{\partial}{\partial z}(D_z\frac{\partial \tilde{c}}{\partial z}) = 0 \quad 6.22$$

From now on, for the purpose of simplicity, the tilde indicating time average is omitted, equation 6.22 is rewritten as

$$\frac{\partial c}{\partial t}+\frac{\partial}{\partial x}(uc)+\frac{\partial}{\partial y}(vc)+\frac{\partial}{\partial z}(wc)-\frac{\partial}{\partial x}(D_x\frac{\partial c}{\partial x})-\frac{\partial}{\partial y}(D_y\frac{\partial c}{\partial y})-\frac{\partial}{\partial z}(D_z\frac{\partial c}{\partial z}) = 0 \quad 6.23$$

All the governing equations have been presented so far. Next those equations will be further simplified for practical uses. As only the convection-diffusion equation will be used for the establishment of water quality models in this study, the simplification is done on this equation solely. For the similar simplification on the Reynold's equations, these books(Newman, 1970; Ippen, 1966) provide more detailed accounts. It is true that a three dimensional model can represent a prototype situation fully. However, it may not be always necessary to use a three dimensional representation if fewer dimensions are adequate to represent the prototype. In estuary cases, when a complete mixing exists either laterally or vertically or both, two or one dimensional models are enough to describe the change of water parameters in those estuaries. For a laterally (supposing y direction) complete mixing estuary, the laterally averaged equation of convection-dispersion is

$$\frac{\partial}{\partial t}(Bc) + \frac{\partial}{\partial x}(uBc) + \frac{\partial}{\partial z}(wBc) - \frac{\partial}{\partial x}(BE_x\frac{\partial c}{\partial x}) - \frac{\partial}{\partial z}(BD_z\frac{\partial c}{\partial z}) = 0 \qquad 6.24$$

where B = the width of an estuary

E_x = the coefficient of longitudinal dispersion

For a vertically (supposing z direction) complete mixing estuary, the vertically averaged equation of convection - dispersion is

$$\frac{\partial}{\partial t}(Hc) + \frac{\partial}{\partial x}(uHc) + \frac{\partial}{\partial y}(wHc) - \frac{\partial}{\partial x}(HE_x\frac{\partial c}{\partial x}) - \frac{\partial}{\partial y}(HD_y\frac{\partial c}{\partial y}) = 0 \qquad 6.25$$

where H = the depth of an estuary

E_x = the coefficient of longitudinal dispersion

For a cross sectionally complete mixing estuary, the cross sectionally averaged one dimensional equation of convection - dispersion is

$$\frac{\partial}{\partial t}(Ac) + \frac{\partial}{\partial x}(uAc) - \frac{\partial}{\partial x}(AE_x\frac{\partial c}{\partial x}) = 0 \qquad 6.26$$

where A = the cross section area

E_x = the coefficient of longitudinal dispersion

It should be pointed out that all forms of convection - diffusion/dispersion equations are derived only for conservative solutes, otherwise, source and sink terms must be added to these equations for non-conservative solutes such as BOD and DO.

6.3 Galerkin Formulation

The finite element method has been introduced previous in chapter 5. After presenting the governing equations in section 6.2, the finite element method can now be applied to these equations forming mathematical models. In this section, a detailed formulation for applying the Galerkin-finite element method into River Tees will be presented.

There are four types of convection-diffusion/dispersion equations (6.23 - 6.26) as seen in the last section. As the River Tees is a partially mixed narrow estuary, the laterally integrated two dimensional equation 6.24 is chosen for the model formulation. The particular finite element method to be used for the formulation is the Galerkin method for it is widely used in many cases. From the procedures of using the finite element method outlined in section 5.5, the type of finite elements and the form of shape functions should be selected first. In two dimensional cases, either quadrilateral or triangular elements are used to subdivide the whole solution domain, and bilinear functions are used for shape functions. For ease of computation, the different shape and size of elements in the global coordinates(X,Y) are transformed into the same size of square elements in the local coordinates(ξ, η), illustrated in Fig 6.1

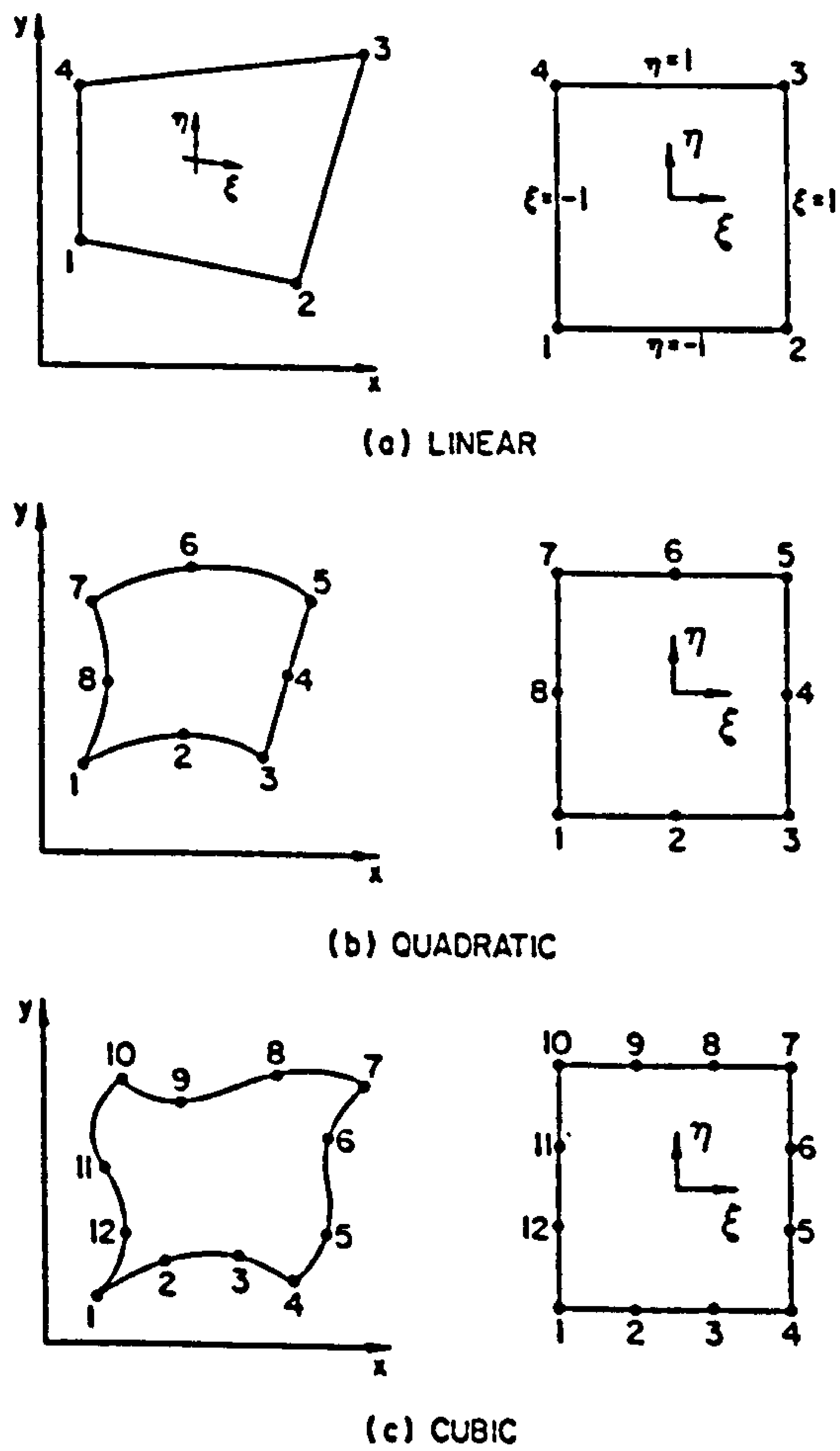


Fig. 6.1 (a) Linear, (b) quadratic and (c) cubic isoparametric elements in local and global coordinates (After Pinder, 1977)

Thus, the global coordinates are expressed in terms of the local coordinates by

$$X = X(\xi, \eta)$$

$$Y = Y(\xi, \eta)$$

The numerical solution for c is approximated in element e by

$$c^e = \sum_{i=1}^{4} N_i^e c_i^e$$

N_i^e is defined as a shape function which has unit value at the corresponding node and zero values at all other nodes.

If the transformation functions take the form as

$$X(\xi, \eta) = \sum_{i=1}^{4} N_i^e X_i^e$$

$$Y(\xi, \eta) = \sum_{i=1}^{4} N_i^e Y_i^e$$

i.e., the shape functions which interpolate the nodal variables are also used to transform the coordinates, then the elements are called isoparametric. An important advantage of isoparametric element calculation is the similarity between the calculations of different elements.

For the linear isoparametric quadrilateral element as shown in Fig.6.1, the shape functions can be shown to have the form in the local coordinate system (Pinder and Gray, 1977)

$$N_1 = \frac{1}{4}(1-\xi)(1-\eta)$$

$$N_2 = \frac{1}{4}(1+\xi)(1-\eta)$$

$$N_3 = \frac{1}{4}(1+\xi)(1+\eta)$$

$$N_4 = \frac{1}{4}(1-\xi)(1+\eta)$$

For the convenience of the formulation, the equation 6.24 is rewritten by assuming a constant width B as

$$R(c,x,z) = \frac{\partial}{\partial x}(E_x\frac{\partial c}{\partial x}) - u\frac{\partial c}{\partial x} + \frac{\partial}{\partial z}(D_z\frac{\partial c}{\partial z}) - w\frac{\partial c}{\partial z} - \frac{\partial c}{\partial t} = o$$

when the exact solution c is replaced by the numerical solution $\tilde{c}$ in the form of nodal variables and interpolation functions as

$$c(x,z,t) \approx \tilde{c}(x,z,t) = \sum_{j=1}^{N} c_j(t)b_i(x,z)$$

where

N = the total number of nodes

b_j = the basis function corresponding to the node j, which is an assemble of shape functions of adjacent elements, $b_j : \{N^j_{j_1}, N^j_{j_2}, ..., N^j_{j_n}\}$

Then,

$$R(\tilde{c}, x, z) \neq 0$$

which is called the solution residual or error.

The weighted residual method states that

$$\iint R(\tilde{c}, x, z) w_i(x, z) dx\, dz = 0, \qquad i = 1, 2, ..N$$

where $w_i(x, z)$ = the weighting functions

The Galerkin method chooses the interpolation function b_i as its weighting functions, thus

$$\iint R(\tilde{c}, x, z) b_i(x, z) dx\, dz = 0, \qquad i = 1, 2, ..N$$

The above equation is expanded as

$$\iint [\frac{\partial}{\partial x}(E_x \frac{\partial \tilde{c}}{\partial x}) - u\frac{\partial \tilde{c}}{\partial x} + \frac{\partial}{\partial z}(D_z \frac{\partial \tilde{c}}{\partial z}) - w\frac{\partial \tilde{c}}{\partial z} - \frac{\partial \tilde{c}}{\partial t}] b_i dx\, dy = 0 \qquad 6.27$$

Applying Green's theorem to the second order derivative terms in the above integration, they can be written as

$$\iint b_i \frac{\partial}{\partial x}(E_x \frac{\partial \bar{c}}{\partial x}) dx\, dz = \oint_\Gamma b_i E_x \frac{\partial \bar{c}}{\partial x} \vec{n}\, d\Gamma - \iint \frac{\partial b_i}{\partial x} E_x \frac{\partial \bar{c}}{\partial x} dx\, dz$$

$$\iint b_i \frac{\partial}{\partial z}(D_z \frac{\partial \bar{c}}{\partial x}) dx\, dz = \oint_\Gamma b_i D_z \frac{\partial \bar{c}}{\partial z} \vec{n}\, d\Gamma - \iint \frac{\partial b_i}{\partial z} D_z \frac{\partial \bar{c}}{\partial z} dx\, dz$$

Substituting the two terms into equation 6.27, it becomes

$$\begin{aligned} &-\iint [E_x \frac{\partial \bar{c}}{\partial x}\frac{\partial b_i}{\partial x} + u \frac{\partial \bar{c}}{\partial x} b_i + D_z \frac{\partial \bar{c}}{\partial z}\frac{\partial b_i}{\partial z} + w \frac{\partial \bar{c}}{\partial z} b_i + \frac{\partial \bar{c}}{\partial t} b_i] dx\, dz \\ &\quad + \oint_\Gamma b_i E_x \frac{\partial \bar{c}}{\partial x} \vec{n}\, d\Gamma + \oint_\Gamma b_i D_z \frac{\partial \bar{c}}{\partial z} \vec{n}\, d\Gamma = 0 \qquad i = 1,2,3,4 \qquad 6.28 \end{aligned}$$

Since the basic concept of the finite element method is to approximate the solution element by element, from equation 6.28 regardless of the last two terms which will be discussed later, an integration over a typical element e can be expressed

$$\begin{aligned} &\iint_{D_e} \{ \sum_{j=1}^{4} c_j^e [E_x \frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x} + u \frac{\partial N_j}{\partial x} N_i + D_z \frac{\partial N_j}{\partial z}\frac{\partial N_i}{\partial z} + w \frac{\partial N_j}{\partial z} N_i] \\ &\quad + \sum_{j=1}^{4} \frac{dc_j^e}{dt} N_i N_j \} dx\, dz = 0 \qquad i = 1,2,3,4 \qquad 6.29 \end{aligned}$$

where

D_e = area of an element

If further approximations are made for the time derivative term and the instantaneous concentration term as

$$\frac{dc_j^e(t)}{dt} = \frac{c_j^e[(n+1)\Delta t] - c_j^e[(n)\Delta t]}{\Delta t}$$
$$= \frac{c_j^e(n+1) - c_j^e(n)}{\Delta t}$$

$$c_j^e(t) = \alpha c_j^e[(n+1)\Delta t] + (1-\alpha)c_j^e[(n)\Delta t]$$
$$= \alpha c_j^e(n+1) + (1-\alpha)c_j^e(n) \qquad 0 \le \alpha \le 1$$

Equation 6.29 can be written as

$$\iint_{D_e}\{\sum_{j=1}^{4} c_j^e(n+1)[\alpha(E_x\frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x} + u\frac{\partial N_j}{\partial x}N_i + D_z\frac{\partial N_j}{\partial z}\frac{\partial N_i}{\partial z} + w\frac{\partial N_j}{\partial z}N_i)$$
$$+ \frac{1}{\Delta t}N_iN_j]\}dx\,dz$$
$$= \iint_{D_e}\{\sum_{j=1}^{4} c_j^e(n)[(\alpha-1)(E_x\frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x} + u\frac{\partial N_j}{\partial x}N_i + D_z\frac{\partial N_j}{\partial z}\frac{\partial N_i}{\partial z} + w\frac{\partial N_j}{\partial z}N_i)$$
$$+ \frac{1}{\Delta t}N_iN_j]\}dx\,dz \qquad i = 1,2,3,4$$

Because the position of the signs of the summation and integration can be exchanged without affecting the integral, thus the above equation is written as

$$\sum_{j=1}^{4}\{\iint_{D_e}[\alpha(E_x\frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x} + u\frac{\partial N_j}{\partial x}N_i + D_z\frac{\partial N_j}{\partial z}\frac{\partial N_i}{\partial z} + w\frac{\partial N_j}{\partial z}N_i)$$
$$+ \frac{1}{\Delta t}N - iN_j]dx\,dz\}c_j^e(n+1)$$
$$= \sum_{j=1}^{4}\{\iint_{D_e}[(\alpha-1)(E_x\frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x} + u\frac{\partial N_j}{\partial x}N_i + D_z\frac{\partial N_j}{\partial z}\frac{\partial N_i}{\partial z} + w\frac{\partial N_j}{\partial z}N_i)$$
$$+ \frac{1}{\Delta t}N_iN_j]dx\,dz\}c_j^e(n) \quad i = 1,2,3,4 \quad 6.30$$

In a compact form, equation 6.30 may be written as

$$\sum_{j=1}^{4} K^e_{ij} c^e_j(n+1) = \sum_{j=1}^{4} f^e_{ij} c^e_j(n) \qquad i = 1,2,3,4 \tag{6.31}$$

where

$$K^e_{ij} = \iint_{D_e} [\alpha(E_x \frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x} + u\frac{\partial N_j}{\partial x}N_i + D_z\frac{\partial N_j}{\partial z}\frac{\partial N_i}{\partial z} + w\frac{\partial N_j}{\partial z}N_i) + \frac{1}{\Delta t}N_i N_j] dx\, dz$$

$$f^e_{ij} = \iint_{D_e} [(\alpha - 1)(E_x \frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x} + u\frac{\partial N_j}{\partial x}N_i + D_z\frac{\partial N_j}{\partial z}\frac{\partial N_i}{\partial z} + w\frac{\partial N_j}{\partial z}N_i) + \frac{1}{\Delta t}N_i N_j] dx\, dz$$

In a matrix form, equation 6.31 is expressed as

$$\begin{bmatrix} K^e_{11} & K^e_{12} & K^e_{13} & K^e_{14} \\ K^e_{21} & K^e_{22} & K^e_{23} & K^e_{24} \\ K^e_{31} & K^e_{32} & K^e_{33} & K^e_{34} \\ K^e_{41} & K^e_{42} & K^e_{43} & K^e_{44} \end{bmatrix} \times \begin{bmatrix} c^e_1 \\ c^e_2 \\ c^e_3 \\ c^e_4 \end{bmatrix}^{n+1} = \begin{bmatrix} f^e_{11} & f^e_{12} & f^e_{13} & f^e_{14} \\ f^e_{21} & f^e_{22} & f^e_{23} & f^e_{24} \\ f^e_{31} & f^e_{32} & f^e_{33} & f^e_{34} \\ f^e_{41} & f^e_{42} & f^e_{43} & f^e_{44} \end{bmatrix} \times \begin{bmatrix} c^e_1 \\ c^e_2 \\ c^e_3 \\ c^e_4 \end{bmatrix}^{n}$$

To calculate K_{ij} and f_{ij}, it is necessary to transform the integration in global coordinates into the integration in local coordinates. The following relationships can be derived by the chain rule of derivative

$$\frac{\partial N(\xi,\eta)}{\partial x} = \frac{\partial N(\xi,\eta)}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N(\xi,\eta)}{\partial \eta}\frac{\partial \eta}{\partial x}$$

$$\frac{\partial N(\xi,\eta)}{\partial z} = \frac{\partial N(\xi,\eta)}{\partial \xi}\frac{\partial \xi}{\partial z} + \frac{\partial N(\xi,\eta)}{\partial \eta}\frac{\partial \eta}{\partial z}$$

and

$$\frac{\partial \xi}{\partial x} = \frac{1}{[J]}\frac{\partial z}{\partial \eta}$$

$$\frac{\partial \eta}{\partial x} = -\frac{1}{[J]}\frac{\partial z}{\partial \xi}$$

$$\frac{\partial \xi}{\partial z} = -\frac{1}{[J]}\frac{\partial x}{\partial \eta}$$

$$\frac{\partial \eta}{\partial z} = \frac{1}{[J]}\frac{\partial x}{\partial \xi}$$

$$dx\, dy = [J]d\xi\, d\eta$$

where

$$[J] = det\begin{vmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} \end{vmatrix}$$

Substituting these relationships into the expressions of K_{ij}^e and f_{ij}^e, they become

$$\begin{aligned} K_{ij}^e = \int_{-1}^{1}\int_{-1}^{1}\{\alpha[E_x(&\frac{\partial N_i}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_i}{\partial \eta}\frac{\partial \eta}{\partial x})(\frac{\partial N_j}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_j}{\partial \eta}\frac{\partial \eta}{\partial x}) \\ &+ uN_i(\frac{\partial N_j}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_j}{\partial \eta}\frac{\partial \eta}{\partial x}) \\ &+ D_z(\frac{\partial N_i}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_i}{\partial \eta}\frac{\partial \eta}{\partial x})(\frac{\partial N_j}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_j}{\partial \eta}\frac{\partial \eta}{\partial x}) \\ &+ wN_i(\frac{\partial N_j}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_j}{\partial \eta}\frac{\partial \eta}{\partial x})] \\ &+ \frac{1}{\Delta t}N_iN_j\}[J]d\xi\, d\eta \end{aligned}$$

$$
\begin{aligned}
f_{ij}^{e} = \int_{-1}^{1}\int_{-1}^{1} \{ & (\alpha - 1)[E_x(\frac{\partial N_i}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_i}{\partial \eta}\frac{\partial \eta}{\partial x})(\frac{\partial N_j}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_j}{\partial \eta}\frac{\partial \eta}{\partial x}) \\
& + uN_i(\frac{\partial N_j}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_j}{\partial \eta}\frac{\partial \eta}{\partial x}) \\
& + D_z(\frac{\partial N_i}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_i}{\partial \eta}\frac{\partial \eta}{\partial x})(\frac{\partial N_j}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_j}{\partial \eta}\frac{\partial \eta}{\partial x}) \\
& + wN_i(\frac{\partial N_j}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial N_j}{\partial \eta}\frac{\partial \eta}{\partial x})] \\
& + \frac{1}{\Delta t}N_iN_j\}[J]d\xi\, d\eta
\end{aligned}
$$

These integral are not at all convenient for analytical evaluation, therefore an approximate calculation must be used. The Gaussian quadrature (Kardestunca, 1987) is commonly used to obtain the results numerically. The lengthy integral above can be written in a general form

$$I = \int_{-1}^{1}\int_{-1}^{1} f(\xi, \eta)d\xi\, d\eta$$

Using the Gaussian quadrature method, the integration is approximated by

$$
\begin{aligned}
I &= \int_{-1}^{1}\int_{-1}^{1} f(\xi, \eta)d\xi\, d\eta \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} H_jH_if(\xi_i, \eta_j)
\end{aligned}
$$

where

n = the number of integration points

H_i, H_j = the weighting coefficients (see Table 6.1)

For each element, its corresponding matrix can be derived as shown above.

Table 6.1 Gaussian Integration Constants for Line Elements

(After Kardestunca, 1987)

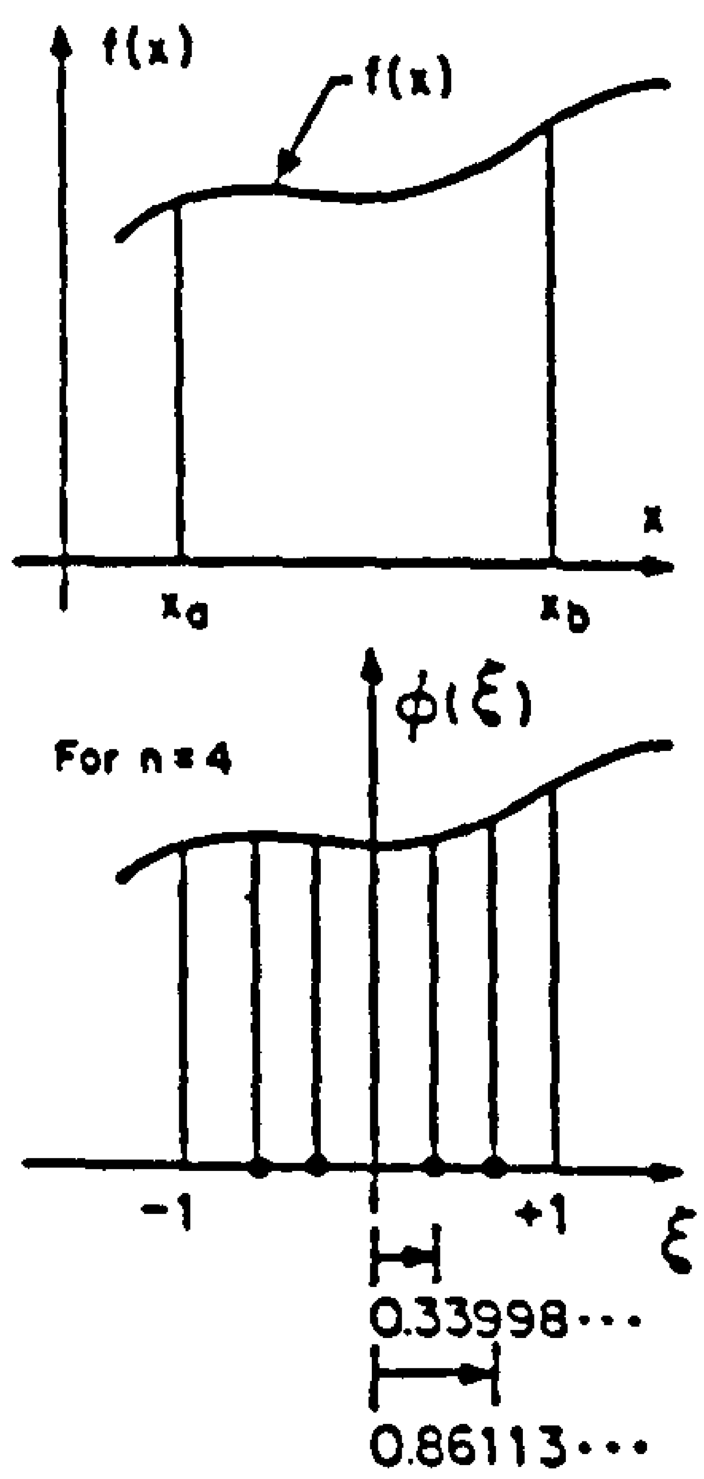


Figure	n†	$\pm\xi_i$	w_i
	1	0.0	2.00000 00000 00000
	2	0.57735 02691 89626	1.00000 00000 00000
	3	0.77459 66692 41483	0.55555 55555 55556
		0.00000 00000 00000	0.88888 88888 88889
	4	0.86113 63115 94053	0.34785 48451 37454
		0.33998 10435 84856	0.65214 51548 62546
	5	0.90617 98459 38664	0.23692 68850 56189
		0.53846 93101 05683	0.47862 86704 99366
		0.00000 00000 00000	0.56888 88888 88889
	6	0.93246 95142 03152	0.17132 44923 79170
		0.66120 93864 66265	0.36076 15730 48139
		0.23861 91860 83197	0.46791 39345 72691
	7	0.94910 79123 42759	0.12948 49661 68870
		0.74153 11855 99394	0.27970 53914 89277
		0.40584 51513 77397	0.38183 00505 05119
		0.00000 00000 00000	0.41795 91836 73469
	8	0.96028 98564 97536	0.10122 85362 90376
		0.79666 64774 13627	0.22238 10344 53374
$I = \int_a^b f(x)\,dx$		0.52553 24099 16329	0.31370 66458 77887
		0.18343 46424 95650	0.36268 37833 78362
$= \int_{-1}^{+1} \phi(\xi)\lvert J\rvert\,d\xi$	9	0.96816 02395 07626	0.08127 43883 61574
		0.83603 11073 26636	0.18064 81606 94857
		0.61337 14327 00590	0.26061 06964 02935
$= \frac{L}{2}\sum_{i=1}^{n} w_i\phi(\xi_i)$		0.32425 34234 03809	0.31234 70770 40003
		0.00000 00000 00000	0.33023 93550 01260
	10	0.97390 65285 17172	0.06667 13443 08688
		0.86506 33666 88985	0.14945 13491 50581
		0.67940 95682 99024	0.21908 63625 15982
		0.43339 53941 29247	0.26926 67193 09996
		0.14887 43389 81631	0.29552 42247 14753

† Answers are exact for polynomials of degree $(2n-1)$ or less; i.e., two integration points are required for a cubic polynomial.

The over-all matrix can be obtained through the coupling relation between nodes.

The last two terms of equation 6.28 have not been included in the derivations. They are actually part of boundary conditions, representing the flux of solute through the boundary. Usually, the two terms are eliminated because of non flux conditions. Otherwise, the flux terms must be quantified for the calculation.

The parameters u, w, E_x, and D_z have not been discussed as for the form of their representation in the formulation. These parameters cannot be expressed as known functions normally, and only their nodal values could be known. But the values of these parameters must be known throughout the solution domain for the calculation. Thus, interpolation should be used for that purpose. In each element the distribution of these parameters can be assumed to vary in the same way as the state variable. The same interpolation functions used for the state variable can be used for the interpolation of these parameters.

6.4 Finite Element Program Structure

Having presented in detail the isoparametric element formulation for the two-dimensional convection-dispersion/diffusion equation, it now remains to express the formulation in the form of a computer program. A FORTRAN language program 'ESTUARY 'has been written on the basis of the formulation. The program flow chart gives the order of the computation.

The computation described in the flow chart is performed by a main program and a few subroutines. The main program reads in all the model parameters and starts to solve the problem in time increment. The subroutine MESH is first called by the main program. MESH performs the numbering of nodes and elements according to the required number of nodes in X, Y directions. The numbering of nodes should be along the direction which is assigned the least number of elements. In this way the bandwidth of the global matrix is minimized. The bandwidth is equal to one plus the maximum of the difference between the largest and smallest node numbers in an element. Next, the subroutine MATRIX is called during the time loop of the main program. MATRIX performs the calculation of element matrix and the assembly of over-all matrix, during which the subroutine TRANSF is called. TRANSF is a subroutine to transfer all the calculations into local coordinate system. Finally, the subroutine GAUSS is called to solve the overall finite element matrix. GAUSS uses the Gaussian elimination method to solve the system of equations for nodal values. The whole program is written in a way to be as simple and straightforward as possible, and all the signs appearing in the program are explained when they are used.

start

input data: mesh size
dispersion and diffusion coefficients
initial conditions
numerical parameters

start of time loop

initializing arrays

read: boundary conditions
nodal coordinates
nodal velocities

calculate element matrix
assemble element matrix

solve overall equations
by Gaussian elimination method

output solutions

end of time loop

Fig. 6.2 The Flow Chart of the Program ESTUARY

Chapter 7 Kriging-Finite Element Modelling of Water Quality

7.1 Introduction

A description of the mathematical formulation for the two-dimensional water quality model has been presented in the previous chapter. In this chapter, the model is applied to the River Tees so that it can be verified as a useful prediction or planning tool.

As could be seen from the model formulation of last chapter, a lot of data/parameters need be prepared before running a model. These data include flow fields, coefficients of dispersion and diffusion, boundary and initial conditions. The following sections will discuss how to specify each item of the data as model input. Then the model is used to simulate salinity intrusions using field data, followed by the interpretation and analysis of the simulation results.

7.2 The River Tees and Its Element Mesh

The estuary of the River Tees is located in the north east of England. Its water quality has been affected by the discharge of wastes from domestic and industrial sources. To investigate the pollution level caused by the waste load entering the estuary, a mathematical model is an ideal mean for the purpose of much a study. To model an estuary, its physical properties should be fully known.

Several authors (Lewis, 1979, 1981, 1983; Farraday, 1973, etc.) have given descriptions of the Tees estuary. However, a brief account of the estuary is described below.

The River Tees rises in the hills of North Yorkshire and flows eastwards in a wandering course between the industrial concurbations of Stockton and Middlesbrough before finally discharging into the North sea. The estuary has a maximum width and depth of 700 m and 15 m respectively at the mouth. There exists a relatively regular cross-section at the seaward end because of dredging of the main shipping channel. Its tidal limit is at Middleton St. George, which is approximately 44 km from the estuary mouth. Within the tidal limit, the only major tributary is the River Leven which flows into the River Tees 9.7 km upstream of Victoria Bridge. The intrusion of salt water reaches at maximum about 26 km from the mouth(Fig. 7.1). Within this region of salt water penetration, the water surface can be regarded as almost horizontal (Bassindele, 1943).

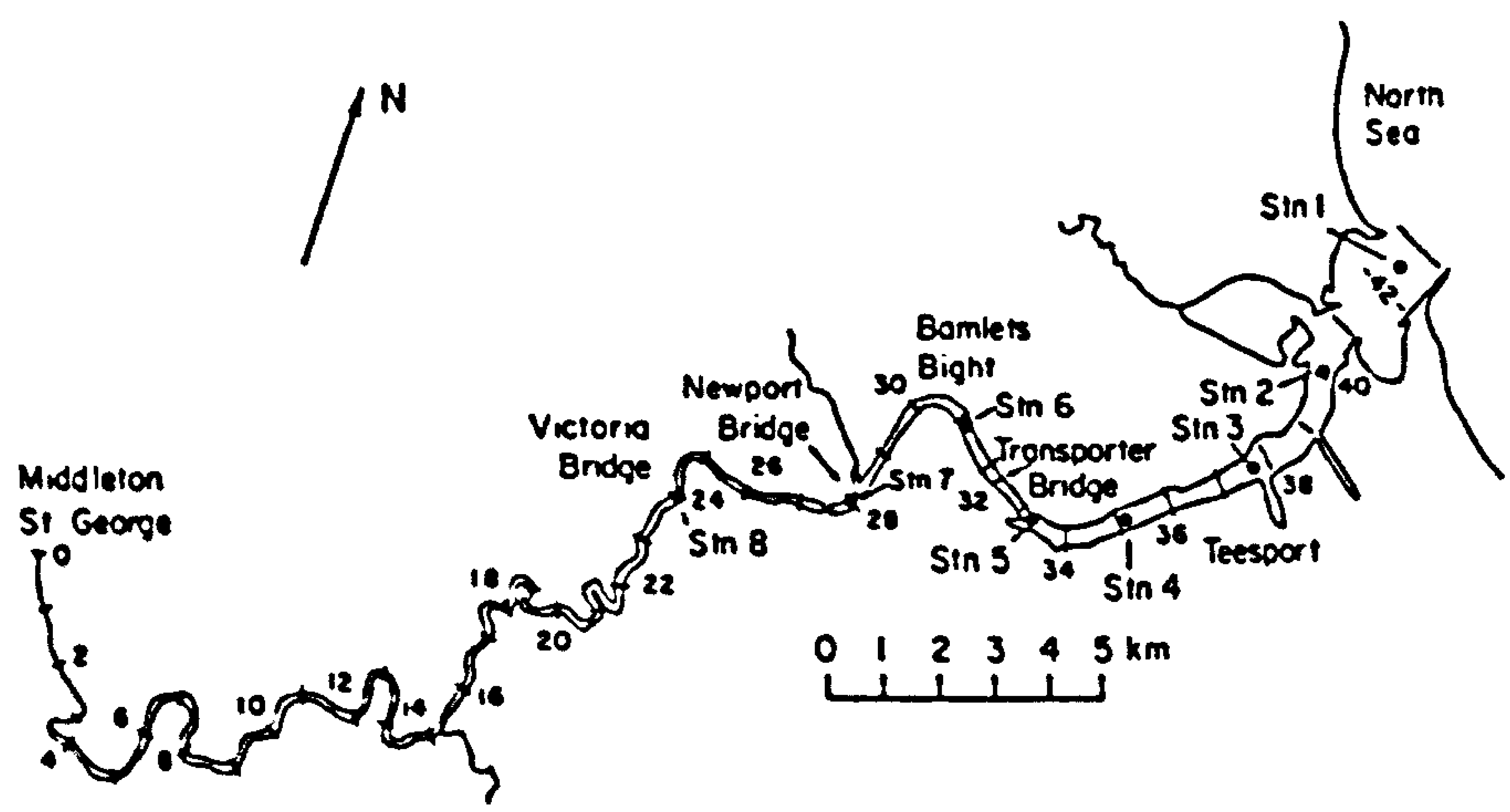


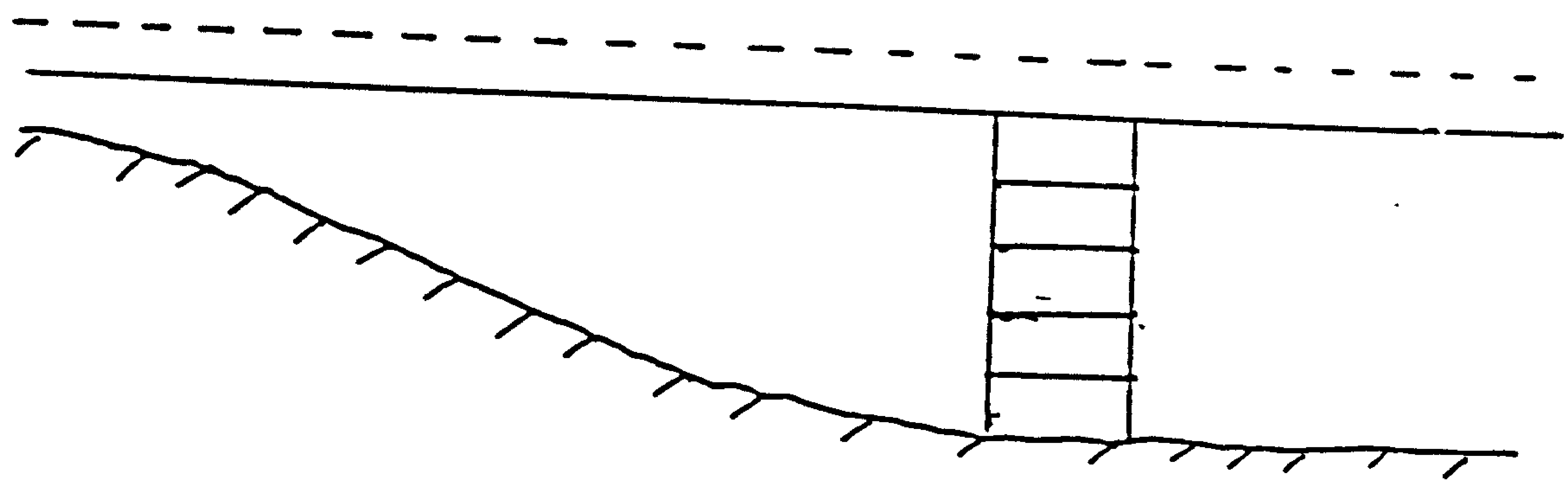
Fig. 7.1 The Estuary of The River Tees (After Lewis, 1983)

The estuary receives an average annual fresh water inflow about $20m^3/s$. This varies from $2m^3/s$ to $70m^3/s$ according to weather conditions. The tide at the mouth is semi-diurnal with mean spring and neap ranges of 4.6 m and 2.3 m respectively. Previous surveys indicate that there exist significant differences of salinity between the surface and bottom. The estuary is classified as partially stratified (Farraday, 1973; Lewis, 1979).

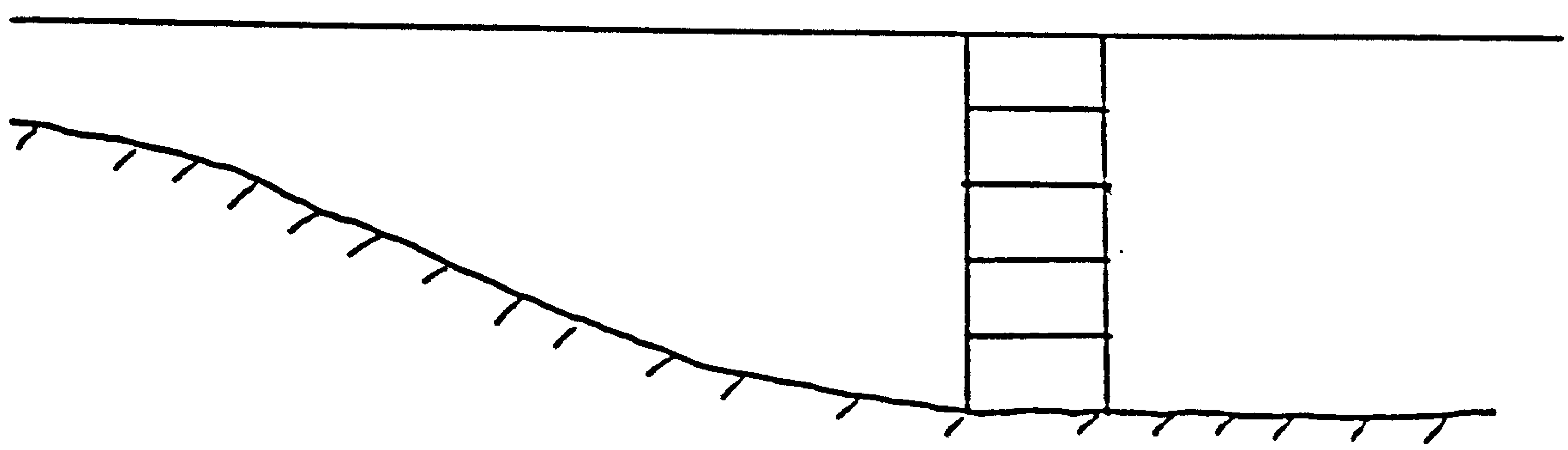
The specification of the finite element mesh is an important part of a finite element model. It was seen in the previous chapter that there are several types of elements available. Quadrilateral elements having a linear interpolation along the element sides are commonly used in practice, thus they are used in this model. In most cases, solution domains are fixed, so once a solution mesh is specified, it could be fixed and be used all the time. In estuary modelling, the water surface may rise or fall because of the tidal effect. The solution domain varies with time. Hence, a fixed mesh cannot represent this characteristic. One way of allowing the domain variation is to let the mesh move with the flow velocity. In this case, the mesh expands or contracts according to the change of the solution domain. As the estuarine solution domain only changes vertically, the mesh only needs to move with the vertical velocity of water.

The mixed Eulerian-Lagrangian mesh(Farraday, 1977) is used for the above particular specification of the solution mesh. This method divides the vertical plane into vertical sections which are fixed longitudinally, then each section is divided into columns of elements which are allowed to expand or contract with the rise or fall of the water surface (Fig. 7.2)

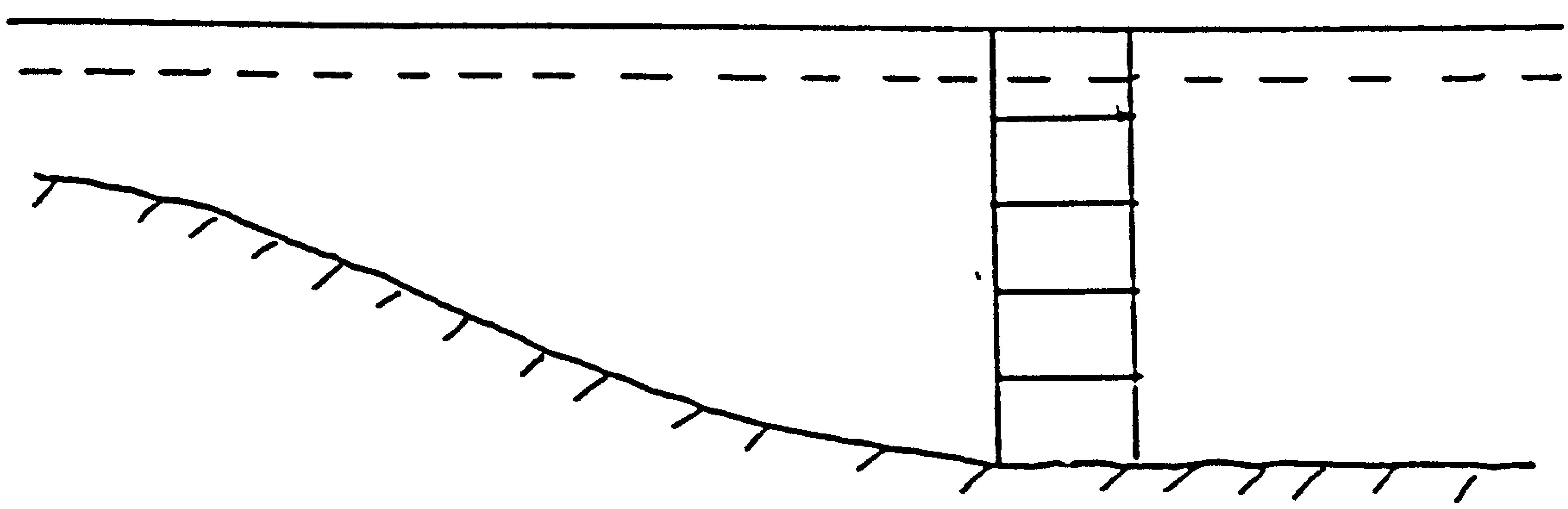
Nodal velocities are set to change linearly at the rate of change of surface elevation at the surface to zero at the river bed. These nodal velocities might be different from vertical water velocities, but the former may be assumed to



(a) At low water



(b) At mid tide



(c) At high water

Fig. 7.2 A Schematic Mesh Net

be an approximation to the latter. As a result, the vertical velocities used in the convection-dispersion equation ought to be modified as velocities relative to the moving mesh. From the proceeding assumption, the relative velocities become very small so that this term may be neglected in the advection-dispersion equation.

7.3 Flow Field

The mass transport in estuaries is controlled physically by the processes of advection and dispersion. Usually the former plays a more important role in transporting mass. By advection, it means the motion with the water velocity. Therefore, an accurate evaluation of velocity field is essential for a good representation of advection in water quality models.

Estuaries are governed by tidal action at the sea face and by river flow. Tidal rise and fall at the mouth of an estuary and amount of river flow are the two dominant factors to affect estuary flow patterns. Their effects can be complicated due to the irregurarity of an estuary geometry. Other factors including density gradient, wind force, frictional force and Coriolis force play a role in deciding the flow pattern. Thus, the complexity of the problem make a rigorous analysis of flow behaviour impossible. Consequently, various approximate approaches to derive velocity fields have to be sought.

There are various types of approaches used to evaluate velocity fields for water quality models, but they can be summarized under two categories: empirical and numerical. These two groups of approaches are to be reviewed briefly in the following paragraphs. Then their applicability will be discussed and a new approach will be proposed.

Empirical approaches have been frequently used to specify velocity field data. Hobbs(1972) used the specified data of hydrography and fresh-water flow to determine the total volume of water flowing through a particular cross-section during any periods, then distributed the total volume over the depth in proportion to the components of tidal, fresh-water and other drift velocities respectively so that the total velocity field could be specified. Farraday(1975) used the method of harmonic analysis to resolve the field velocity data into its periodic and densimeteric components, then specified empirical functions respectively for both periodic and densimeteric flow. Because of the empirical basis of the methods, it is usually regarded as the crudest approach. These empirical methods are based on assumptions, which may not always be justified. For instance, one basic assumption in Farraday's method is that the residual flows are constant over the tidal cycle. This is never true in reality. Fitting empirical functions sounds like very strightforward, but it is a complicated procedure and is very cumbersome. Consequently, other approaches have been sought.

With the advent of modern computers, especially with ever-increasing computing power, numerical methods such as the finite difference method and the finite element method have found applications in many fields. In estuarine modelling, velocity fields can be determined through the simultaneous solution of the continuity and momentum equations together with appropriate boundary and initial conditions. The numerical two-dimensional hydrodynamic model may be either vertically or laterally averaged. The vertically averaged two-dimensional model has been used to simulate the velocity field in wide and shallow estuaries where the assumption of being vertically mixed is valid. This class of models has been developed and applied since late 60's. The laterally averaged two-dimensional model has been used to simulate the velocity field in narrow and deep estuaries where the assumption of being laterally well mixed is valid.

In contrast to the solution of a vertically averaged two-dimensional model, the solution of a laterally averaged two-dimensional model requires the solution of the coupled salt mass transport equation in order to consider the effect of the gravitational circulation. The solution of the coupled equations of motion and mass transport causes additional computational difficulties. For this reason the development of laterally averaged two-dimensional models was later than that of vertically averaged two-dimensional model. Even though there exist fewer laterally averaged models than vertically averaged models, a number of laterally averaged models have been developed for partially mixed estuaries.

The numerical approach to the solution of velocity fields is normally considered more predictive than the empirical approach since the term "model" gives such an impression. One primary fact should be born in mind while using a model. A model supplies no independent information and the results produced are no better than the information it uses for input. Therefore, the input information of a model must first be predictive if the model results are to be regarded as predictive as well. This requirement may be too difficult to be satisfied because the data information such as boundary conditions and mixing coefficients are usually not available. For example, the surface boundary of a laterally averaged model is specified in terms of wind stress, but the wind stress varies in time and space and can only be determined from the solution of an atmospheric circulation model. It may be seen that it becomes even more difficult to specify a boundary condition than to set up the model itself. Thus, it is inevitable that some parameters or expressions used in a model might be chosen as an afterthought.

It is likely that a calibrated model cannot ensure its predictive capability because the model may contain incorrect mechanisms and the agreement between model predictions and observations could have been obtained through an unrealistic choice of parameter values. Mathematically, a hydrodynamic model solving simultaneously the equations of motion and momentum or salt transport is ideal for the derivation of velocity fields, but its predictive capability leaves much to be desired.

It is usually considered impractical to collect sufficient data to specify velocity fields as it is financially impossible to take measurments at as many locations as required by a water quality model. In order to specify the measured velocity field, one of the approaches as discussed before is to fit theoretical velocity distributions using field velocity data. Another approach is to interpolate velocity values at unmeasured points using velocity values at measured points. However, this approach has not been used so far due to the following factors. Firstly, estuary velocity as a variable changes very irregularly in space and time. Secondly, common interpolation methods such as cubic spline method and least square method are only suitable for those variables with a smooth change. Thirdly, assuming a common interpolation method may be used, but insufficient measurments in space may prevent any possible applications because there should exist minimal measurements on which the interpolation can be based.

Though the change of velocity is quite irregular, it still possesses a certain structure, i.e. the velocity varies vertically and horizontally with a general trend. For example, velocity decreases from the water surface to water bottom. This matches with the concept of regionalized variables which is defined as a variable typical of a phenomenon developing in space and/or time and possessing a certain structure. For the interpolation of this class of variables, there exists a geostatistical method called "Kriging method" which situates the problem within a probabilistic frame. The theory of the Kriging method has been outlined in chapter 3, and the procedures of implementation of the method have been described in chapter 4.

A typical field survey on the River Tees spans from the river mouth in the seaward to the Victorial bridge at the upstream or further upstream. There were two major surveys in 1970 and 1975. The 1970 survey covered a range of 24.3 km with 9 sampling stations. The 1975 survey covered a range of 18.5 km with 8 sampling stations. From the point of interpolation, the more sampling stations are involved, the more accurate the estimations are. So the 1970 survey data should be more ideal to be used for the simulation of salinity intrusion. What is more, it almost covered the range of the intrusion of salt water. Unfortunately, the 1970 data are not as accurate and reliable as the 1975 data because there exist quite obvious measurement discrepencies among the 1970 data. Interpolations are made at each node of all element meshes.

7.4 Dispersion and Diffusion

The last section discussed one of the processes of mass transport: advection. In this section, another process of mass transport will be given and its expressed forms in the model will be discussed. This process of mass transport is dispersion and diffusion which are represented in a water quality model in the form of dispersion and diffusion coefficients.

There are two averaging processes involved in estuarine models as discussed in chapter 6. First, temporal averaging should be used to derive a smoothed velocity and solute concentration. This time averaging process results in a time averaged cross product term. By the analogy of Fick's Law of diffusion, this cross product term is set equivalent to the product of a coefficient times a concentration gradient. The coefficient is defined as turbulent diffusion coefficient. Second, spatial averaging should be used to simplify three dimensional models to two or one dimensional models. This spatial averaging results in a spatial cross product term. By the same analogy, the spatial cross product term is expressed by means of a dispersion coefficient.

The developed River Tees model is a laterally averaged two dimensional model. The lateral averaging produces a longitudinal dispersion due to lateral variations of solute concentrations and longitudinal velocity component. The temporal averaging produces longitudinal and vertical diffusions. The longitudinal diffusion may be neglected in comparison with the longitudinal dispersion which is several order higher, but the vertical diffusion is still accountable due to the fact that the vertical dispersion is almost negligible.

There are two approaches to determine the coefficients of diffusion and dispersion. First, they can be calculated according to their definitions if the required data are available. For longitudinal dispersion coefficients, the formula is

$$D_x = \frac{-\frac{1}{B}\int_0^B u'c'dy}{\frac{\partial \bar{c}}{\partial x}}$$

where u', c' are the deviations of lateral velocity and concentration from width averaged ones $\bar{u}$, $\bar{c}$, and B is the width. For vertical diffusion coefficient, the formula is

$$\xi_z = \frac{-\frac{1}{T}\int_0^T w'c'dt}{\frac{\partial \bar{c}}{\partial z}}$$

where w', c' are the turbulent fluctuations from time averaged values $\bar{w}$, $\bar{c}$, and T is the time interval. This first method is difficult to use because sufficient data must be obtained for the calculation. Second, empirical functions for dispersion and diffusion coefficients are used to estimate their values. There are various forms of empirical functions(see relevant references mentioned in chapter 2). Farraday(1973) redefined a formula for the dispersion coefficient used in one dimensional models for the estimation of longitudinal dispersion coefficient used in the two dimensional model of the River Tees. Then, the data measured at a transverse survey section was used to yield an approximate value of $100,000m^2/hr$. For the vertical diffusion coefficient, Farraday used three different methods to yield an estimation within the range of $0.1\ to\ 1.0m^2/hr$. The coefficients of dispersion and diffusion vary in space and time. The variation can only be determined if sufficient field data measured along the estuary at different time are made available. In practice, the cost of such a sampling scheme makes it financially impossible to collect. Hence, empirical functions are fitted for the variation in space and time by trial and error. As for the input to the Tees model, constant values adapted from Farraday's calculation are ready to be used.

7.5 Boundary and Initial Conditions

A water quality model simulates changes of water quality in a solution domain. The solution domain is framed by the boundaries which interface the solution domain with the surrounding area. The boundaries of an estuary model are:

(1) the water surface which interfaces with the atmosphere

(2) the water bottom which interfaces with the estuary bed

(3) the seaward boundary which interfaces with the sea

(4) the upstream boundary which interfaces with the uptream

The model formulation presented in chapter 6 requires the specification of the state of simulated water parameters along all boundaries, i.e., the boundary conditions. There are two types of boundary conditions. The first type is the concentration prescribed boundary where known concentrations are defined. The second type is the concentration flux prescribed boundary where known concentration fluxes are defined. There may be another type of boundary condition which is a combination of the above two boundary conditions.

In case of salinity simulations, the boundary conditions are straightforward. There is no flux through the water surface and bottom. The boundary conditions seaward and landward may take the form of prescribed concentrations as long as the concentration gradients at the two positions are insignificant.

As the water quality model is time dependent, in the case of salinity simulations, salinity concentrations need to be defined initially at all points in the two dimensional vertical domain. But, salinity concentrations are only known at the eight sampling stations. Interpolations must be made at unknown points. Kriging is a powerful interpolation method. Therefore, it is used to interpolate salinity concentrations at all nodal points of the finite element model at the initial time. An accurate input of initial conditions is vital for the following solutions though its effect may die away with time.

7.6 Simulations and Results

What has been described in this chapter is a theoretical frame work. Whether the model in such a frame works well can only be verified by simulating a practical problem. Thus, a salinity intrusion is chosen for the model simulation.

The set of data to be used for the simulation is from the 1975 survey. In this survey, the observations were made over the periods 2-6 July 1975 and 9-13 July 1975 on neap and spring tides respectively. The set of data covering one tidal cycle on 12 July 1975 was selected to provide velocity data and initial condition data. The data are from observations of spring tides. Because of the limitation of study time, a salinity intrusion at neap tides has not been simulated though it is desirable. For the simulation, the upstream limit was located at Victoria Bridge(station 8 of the 1975 survey). The upstream limit of the simulation was restrained by the upstream position of the survey because the flow fields could not be defined beyond the range of the survey. However, the upstream limit of the model could be set at any positions by model users as long as the data required by the model were available in the model region.

The mesh specification has been presented in section 7.2. Now it only needs to quantify the mesh. The entire vertical elevation is divided into columns at 500 metre intervals, and each column is then divided into five equal quadrilateral elements. For a typical element, it has a fixed horizontal interval of 500 metre but a varying vertical interval approximately in range of 0.5-3.5 meter. The time step used in the model is set equal to 0.5 hr. The coefficients of longitudinal dispersion and vertical diffusion are chosen as 100,000 m^2/hr and 0.5 m^2/hr respectively. The initial time of the simulation is 6:30 hr which is at high water.The whole simulation is run for a tidal cycle of 12 hrs and 30 minutes. The ending time of the simulation is 19:00 hr.

The simulation results are compared with the field measurments. The simulation results are produced at all nodes, but the measurements are only available at sampling points. To compare them with each other on a point to point base, interpolations are made at all corresponding nodes by the kriging method. The comparison between the simulation results and the kriged field measurements yields following points:

(1) at first 3 hrs between 6:30-9:30, the model almost exactly reproduces the salinity distribution both longitudinally and vertically. This is shown in the contour maps(Fig. 7.28-7.33), 3-D maps(Fig. 7.34-7.45), salinity distribution curves(Fig. 7.3-7.8) and listings at one of the time steps(Appendix p.4, time 8:00) showing differences between Kriged and modelled values.The largest difference among the listed values is 1.37 ppm, and is approximately 5% of the Kriged value.

(2) at next two and half hrs between 9:30-12:00, the accuracy of the simulation results starts to deteriorate. This is shown in the contour maps(Fig. 7.46-7.50), salinity distribution curves(Fig. 7.9-7.13) and listings at one of the time steps(Appendix p.4, time 11:00) showing differences between Kriged and simulated values. The largest difference among the listed values is 9.50 ppm, and is approximately 40% of the Kriged value.
(3) at next two hrs between 12:00-14:00, the accuracy of the simulation results starts to improve. This is shown in the contour maps(Fig. 7.51-7.54), salinity distribution curves(Fig. 7.14-7.17). and listings at one of the time steps(Appendix p.4, time 13:00) showing differences between Kriged and simulated values. The largest difference among the listed values is 8.15 ppm and is approximately 40% of the Kriged value.
(4) at the last two time intervals between 14:00-17:00, 17:00-19:00, the simulation results behave in the same way as they do in the above periods 2, 3 respectively. This is shown in the contour maps(Fig. 7.55-7.64) and salinity distribution curves(Fig. 7.18-7.27). and listings at one of the time steps(Appendix p.4, time 15:00,18:00) showing differences between Kriged and simulated values. The largest difference among the listed values at 15:00 is 10.03ppm and is approximately 75% of the Kriged value while the largest difference at the listed values at 18:00 is 9.41 ppm and is approximately 35% of the Kriged value.
(5) although the accuracy of the simulation results varies with time at other regions, the simulation results at the seaward region remain highly accurate all the time. The listings in the Appendix(p.4) showed the differences between Kriged and modelled values were less than 10% of the Kriged values.

One important part of mathematical modelling is how to interpret its results so that further understanding about the model may be derived, which leads to finding which factors affect the accuracy of model results. There are two types of such factors. First, the numerical scheme to solve the partial differential equations affects the accuracy of its solutions as an external factor. Second, the input data required by the model affects the model accuracy as an internal factor. The respective discussions on the two sources of modelling error are presented next.

A numerical scheme includes the choice of a numerical method and the discretization in space and time. In chapter 5, two main numerical methods of finite difference and finite element were described, but the finite element method was recommended as the preferred modelling technique due to its ease of approximating irregular boundaries. After selection of a numerical method, the accuracy of the numerical solutions depends crucially on the discretization.

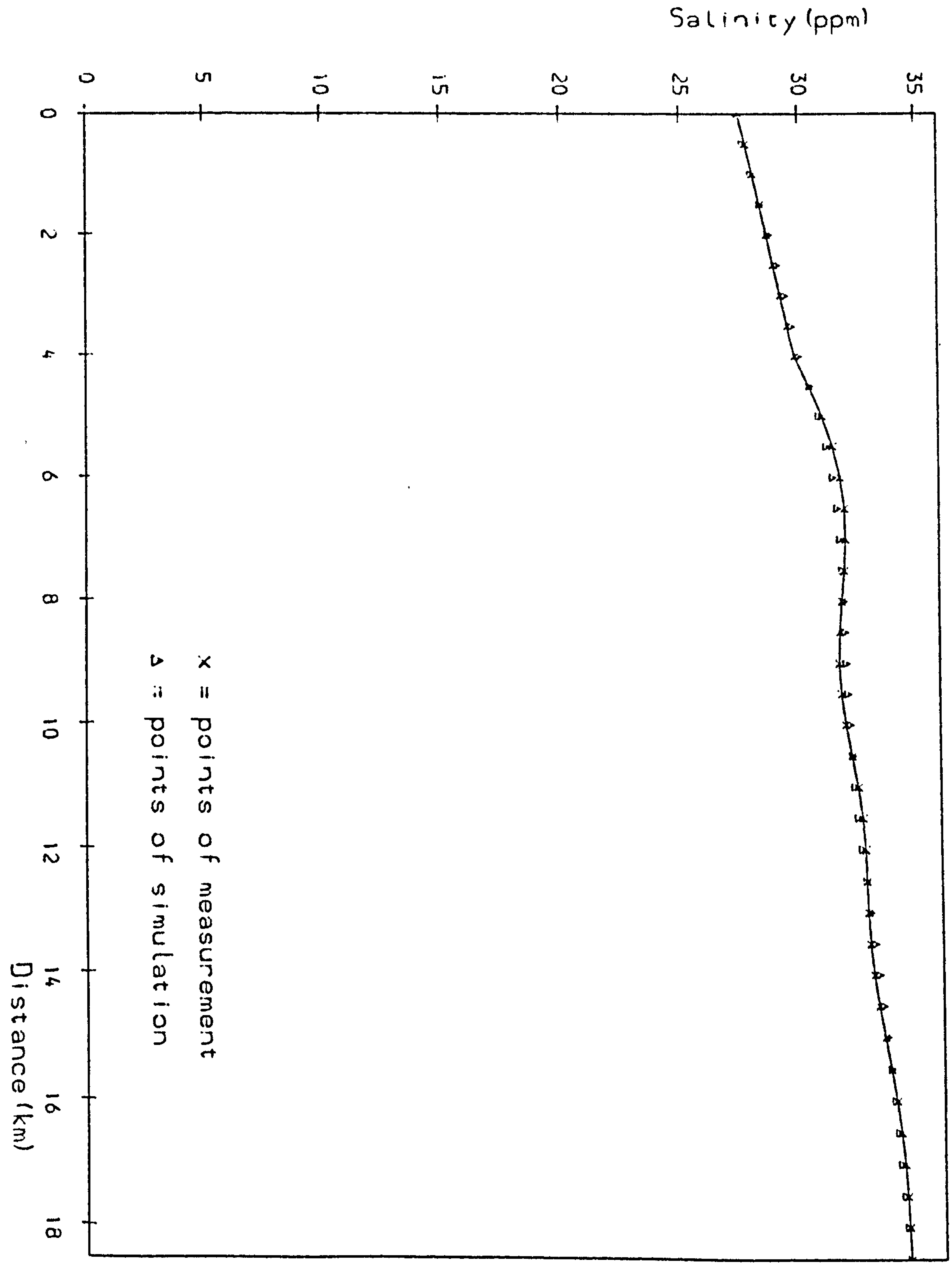


Fig. 7.3 Comparison between measurements and simulations

time=7:00

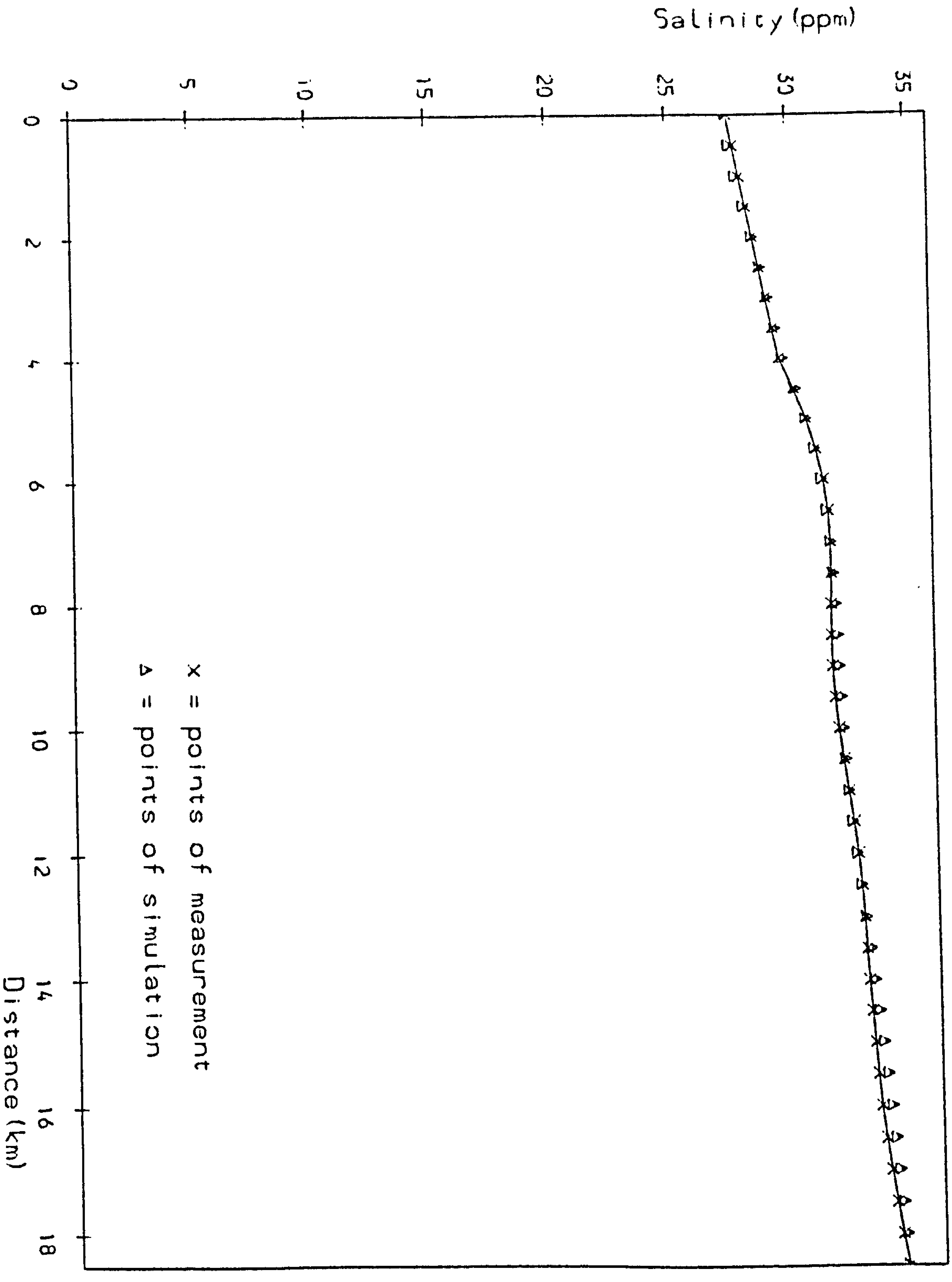


Fig. 7.4 Comparison between measurements and simulations

time=7:30

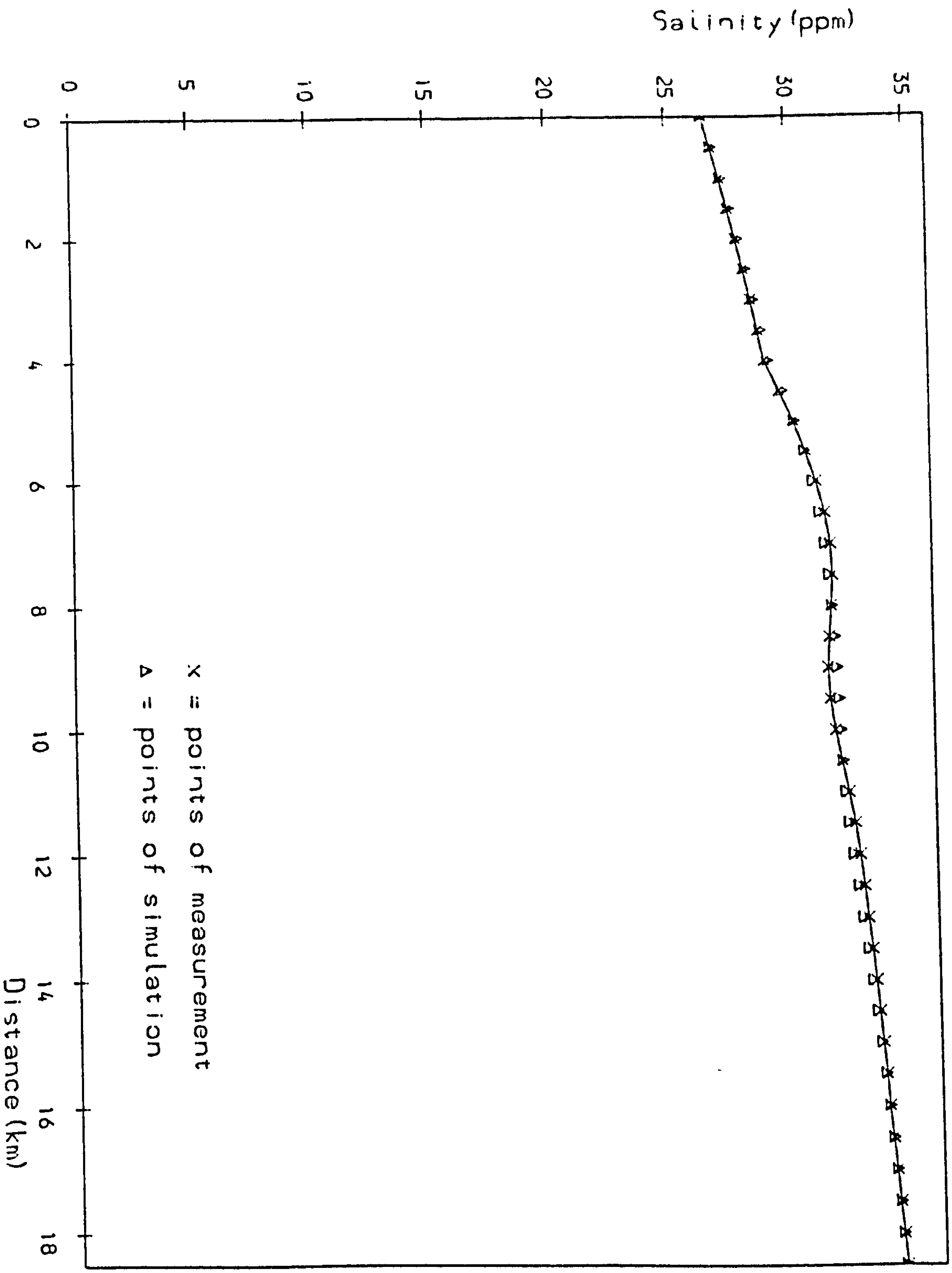


Fig. 7.5 Comparison between measurements and simulations

time=8:00

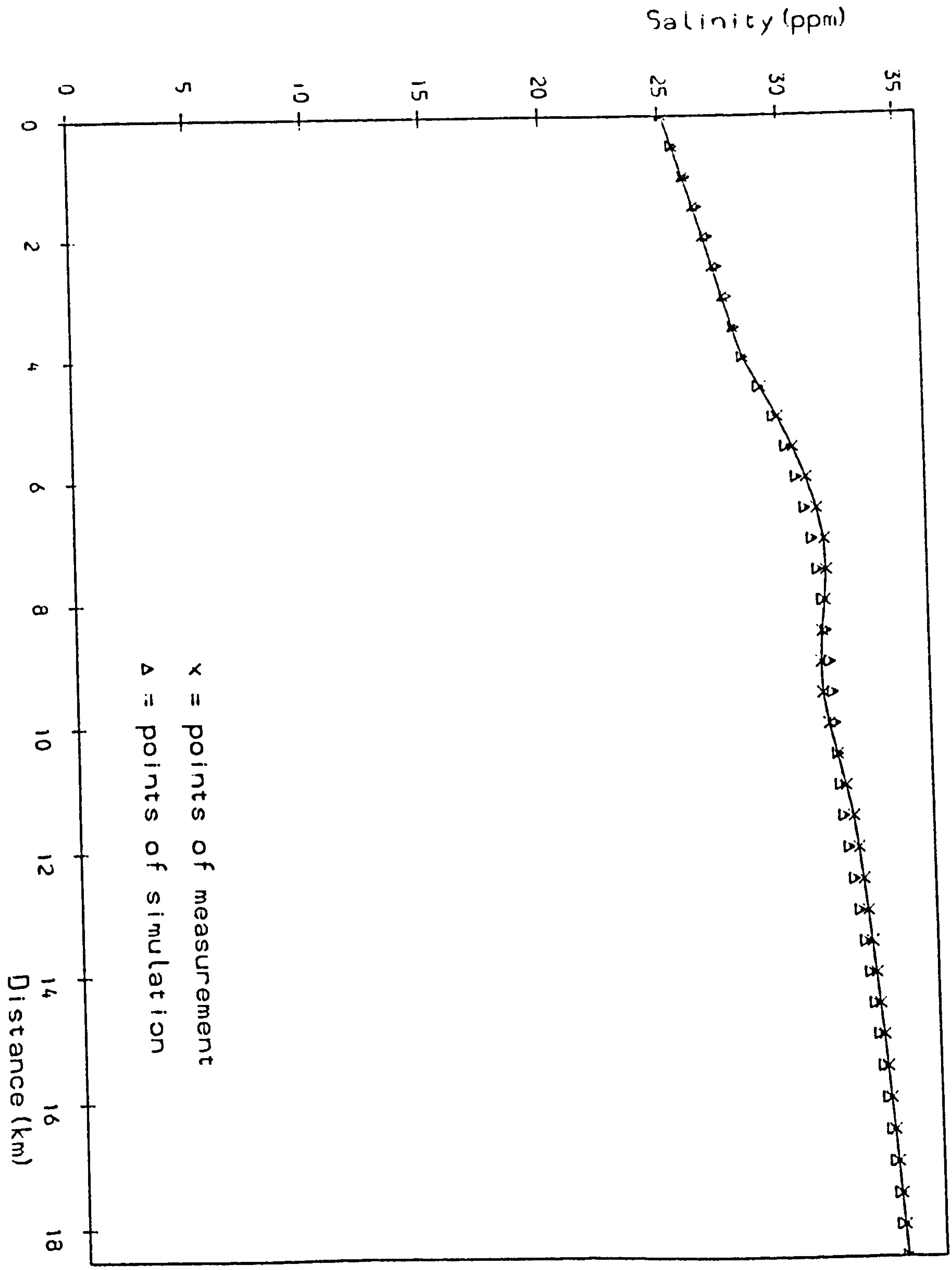


Fig. 7.6 Comparison between measurements and simulations

time=8:30

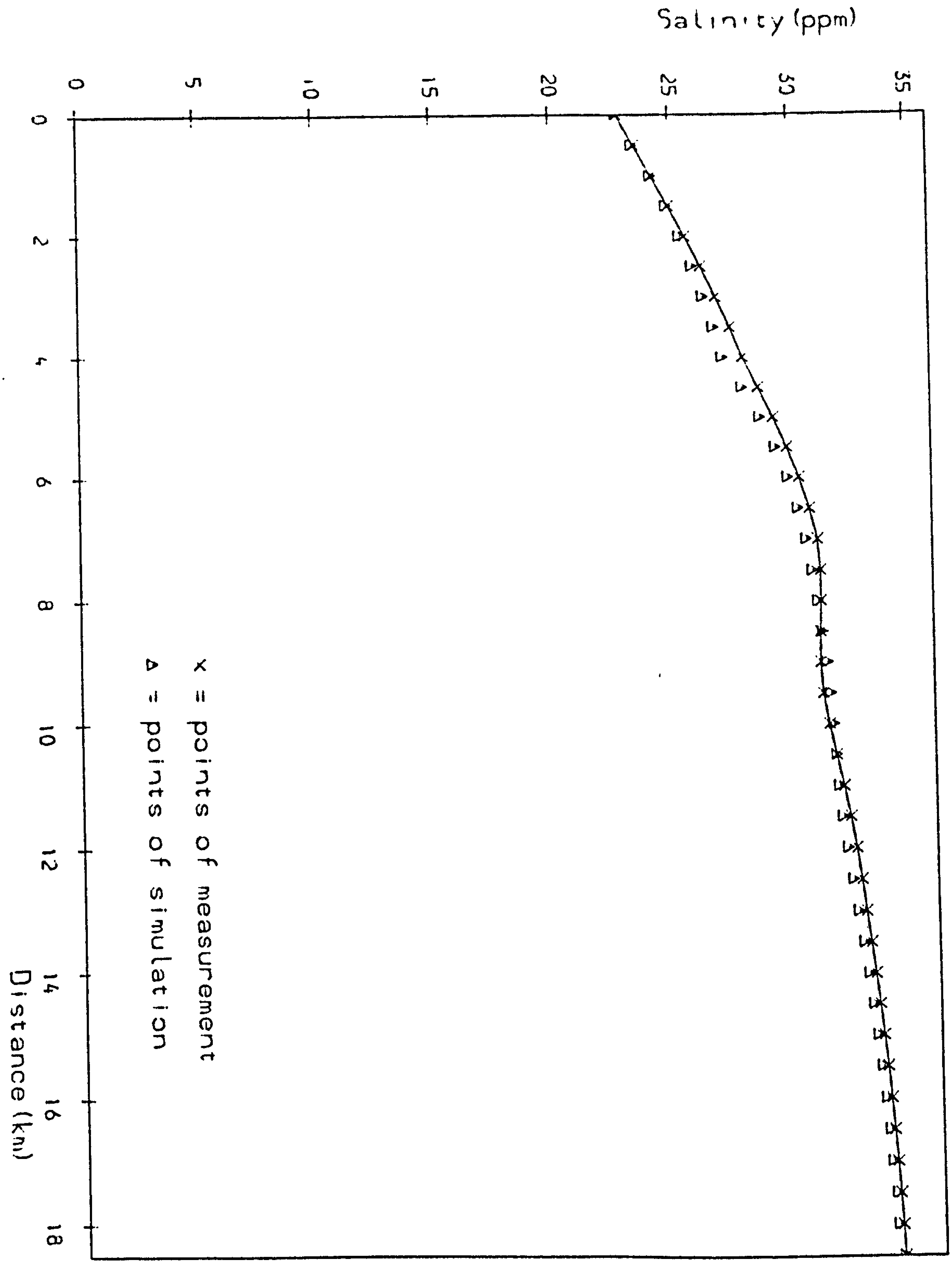


Fig. 7.7 Comparison between measurements and simulations

time=9:00

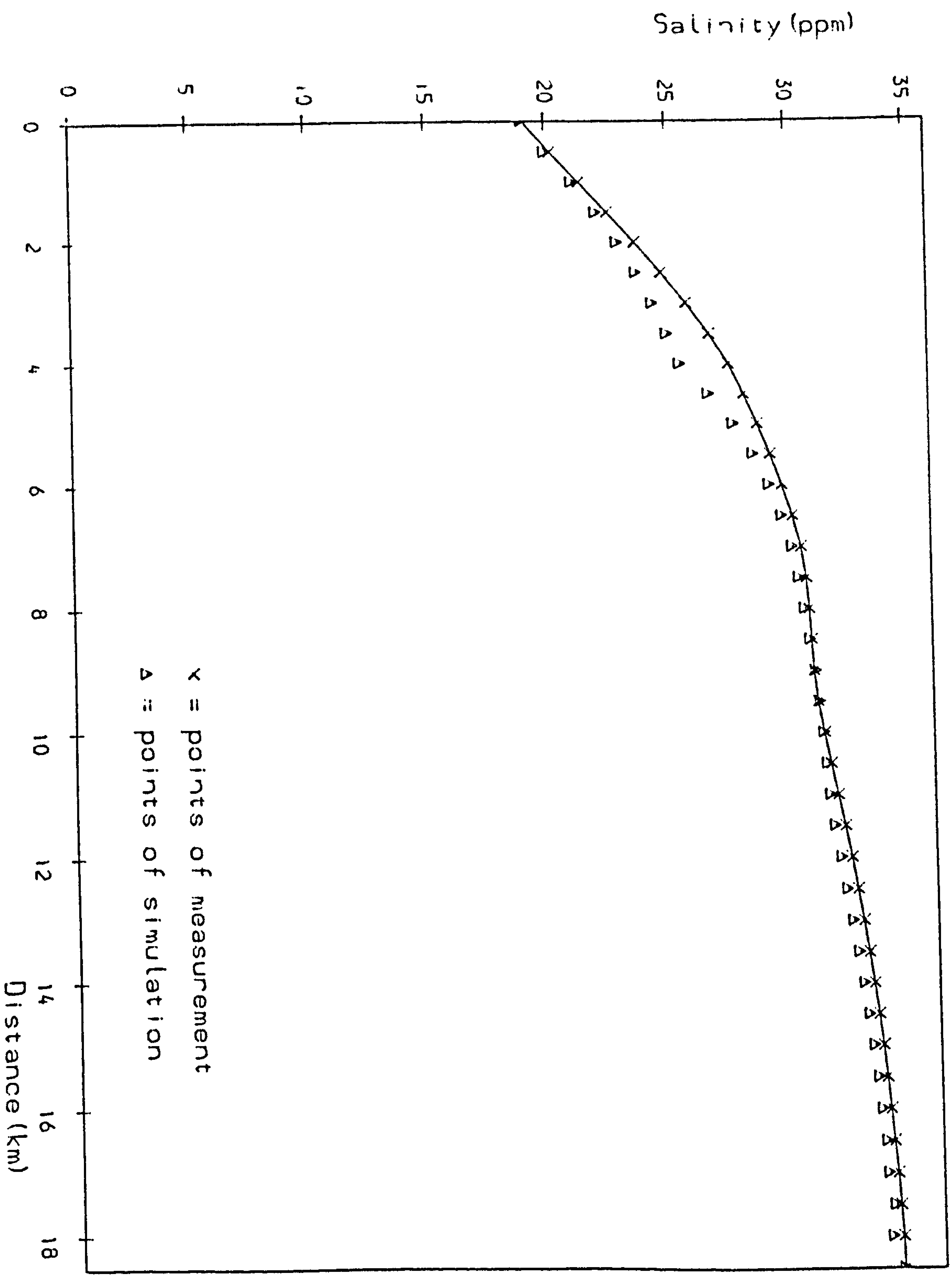


Fig. 7.8 Comparison between measurements and simulations

time=9:30

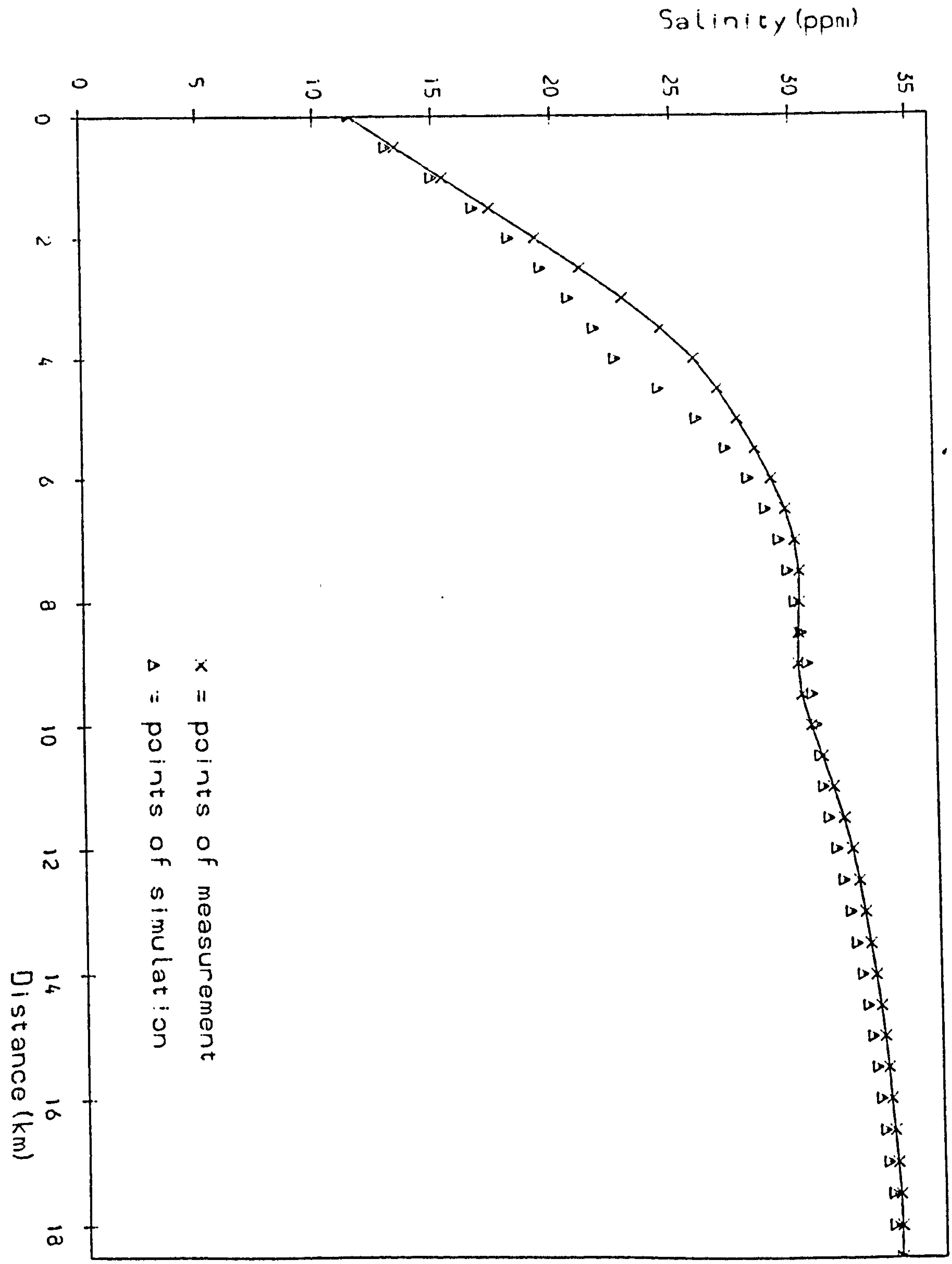


Fig. 7.9 Comparison between measurements and simulations

time=10:00

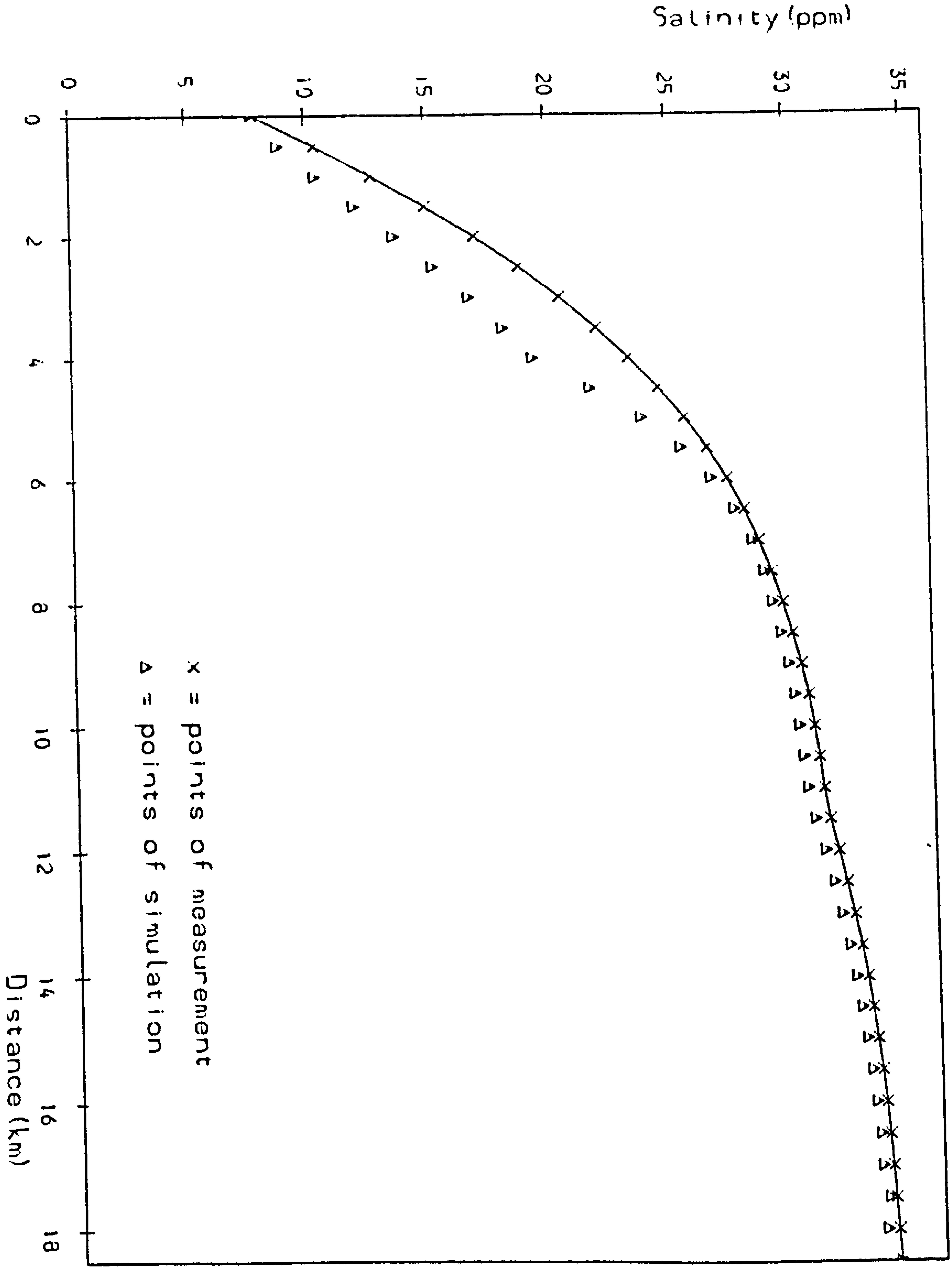


Fig. 7.10 Comparison between measurements and simulations

time=10:30

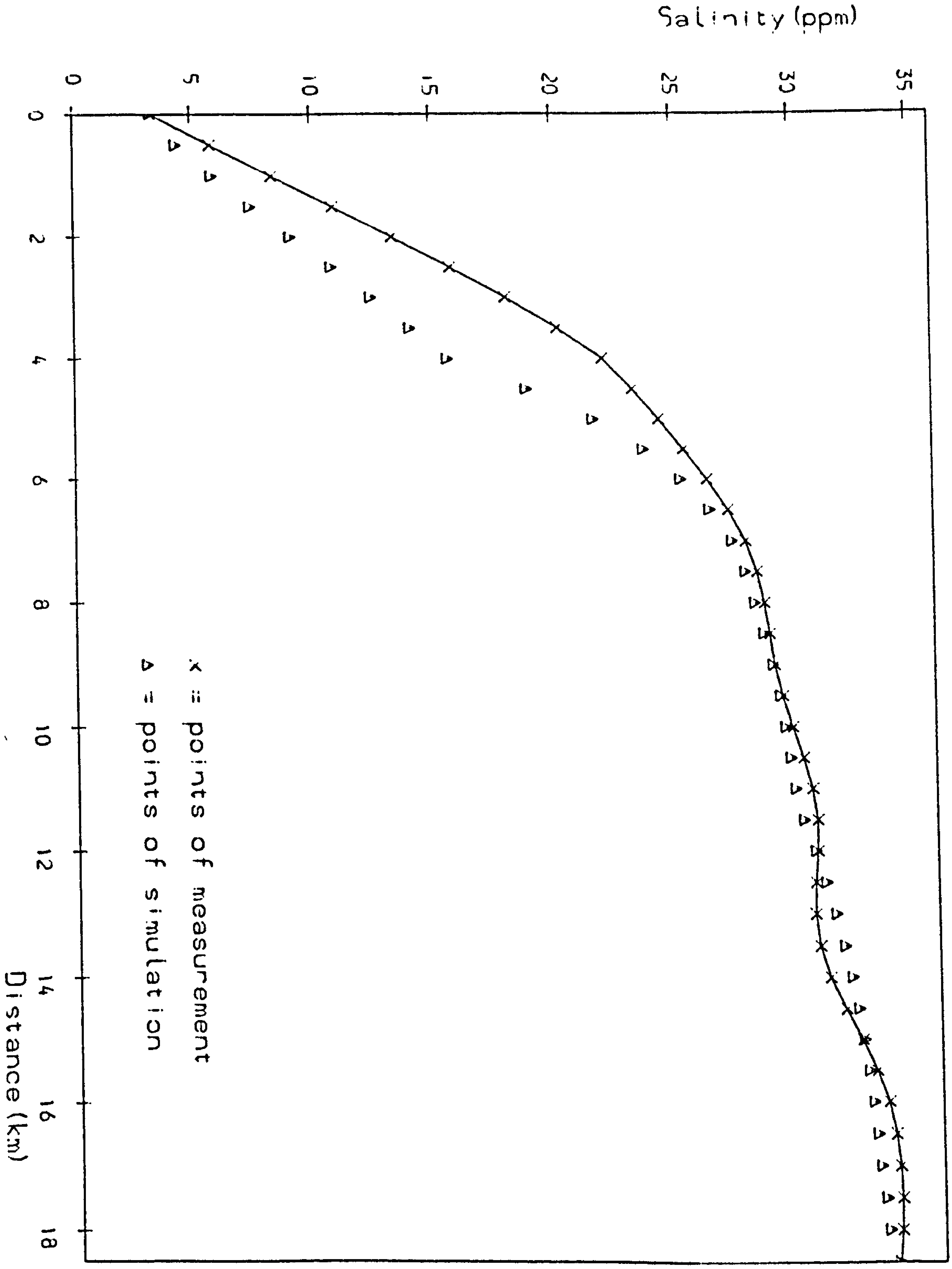


Fig. 7.11 Comparison between measurements and simulations

time=11:00

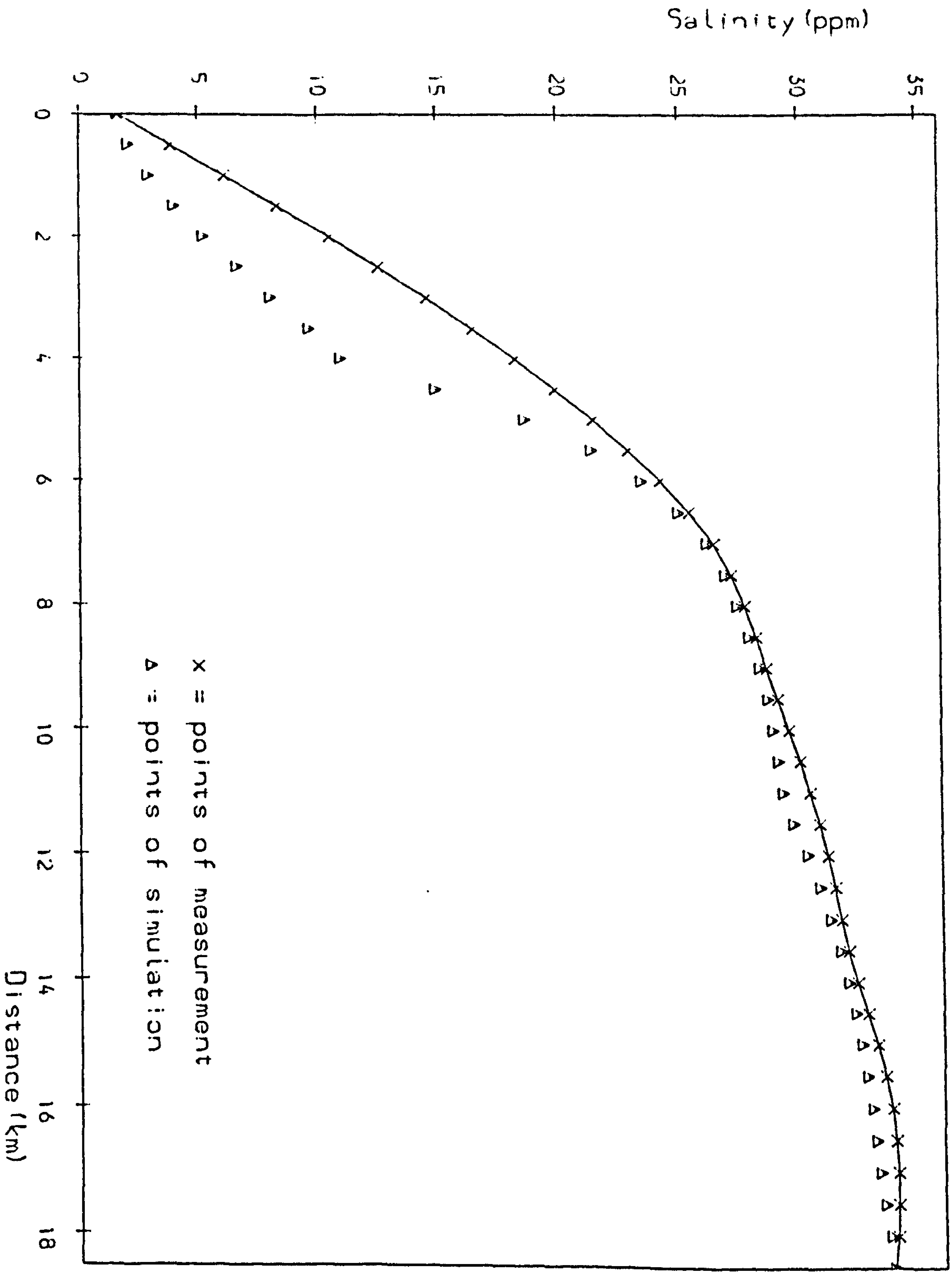


Fig. 7.12 Comparison between measurements and simulations

time=11:30

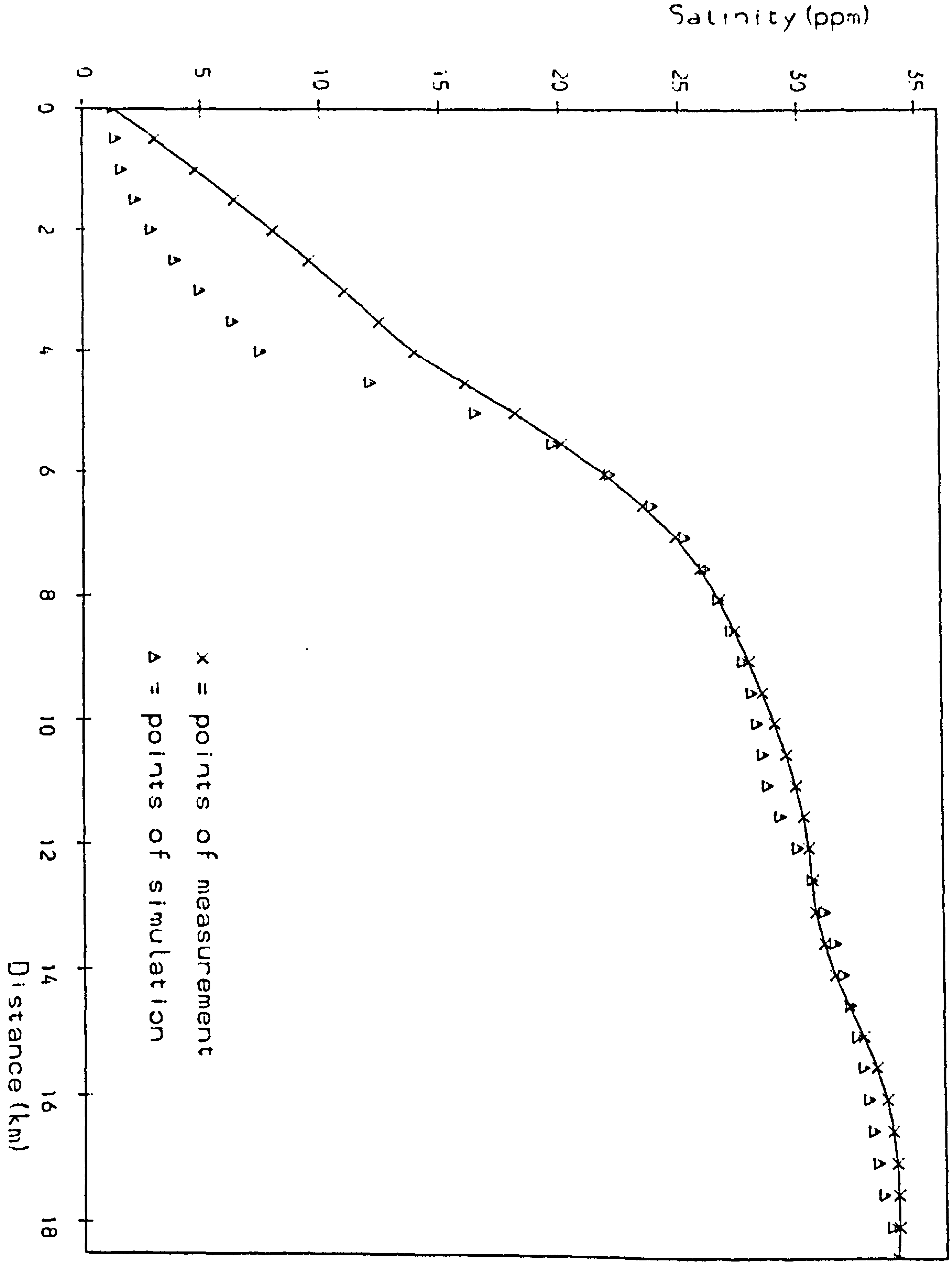


Fig. 7.13 Comparison between measurements and simulations

time=12:00

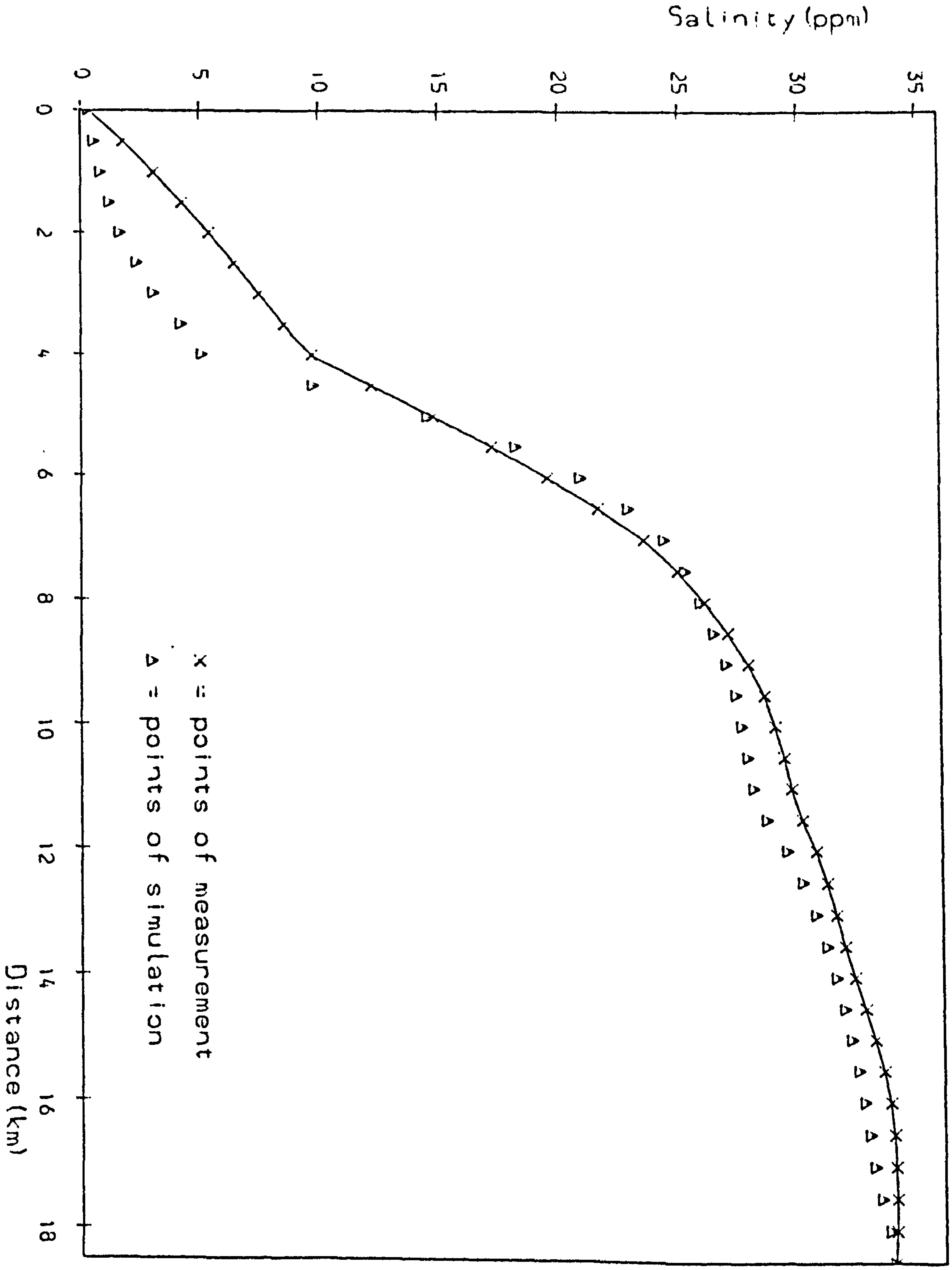


Fig. 7.14 Comparison between measurements and simulations

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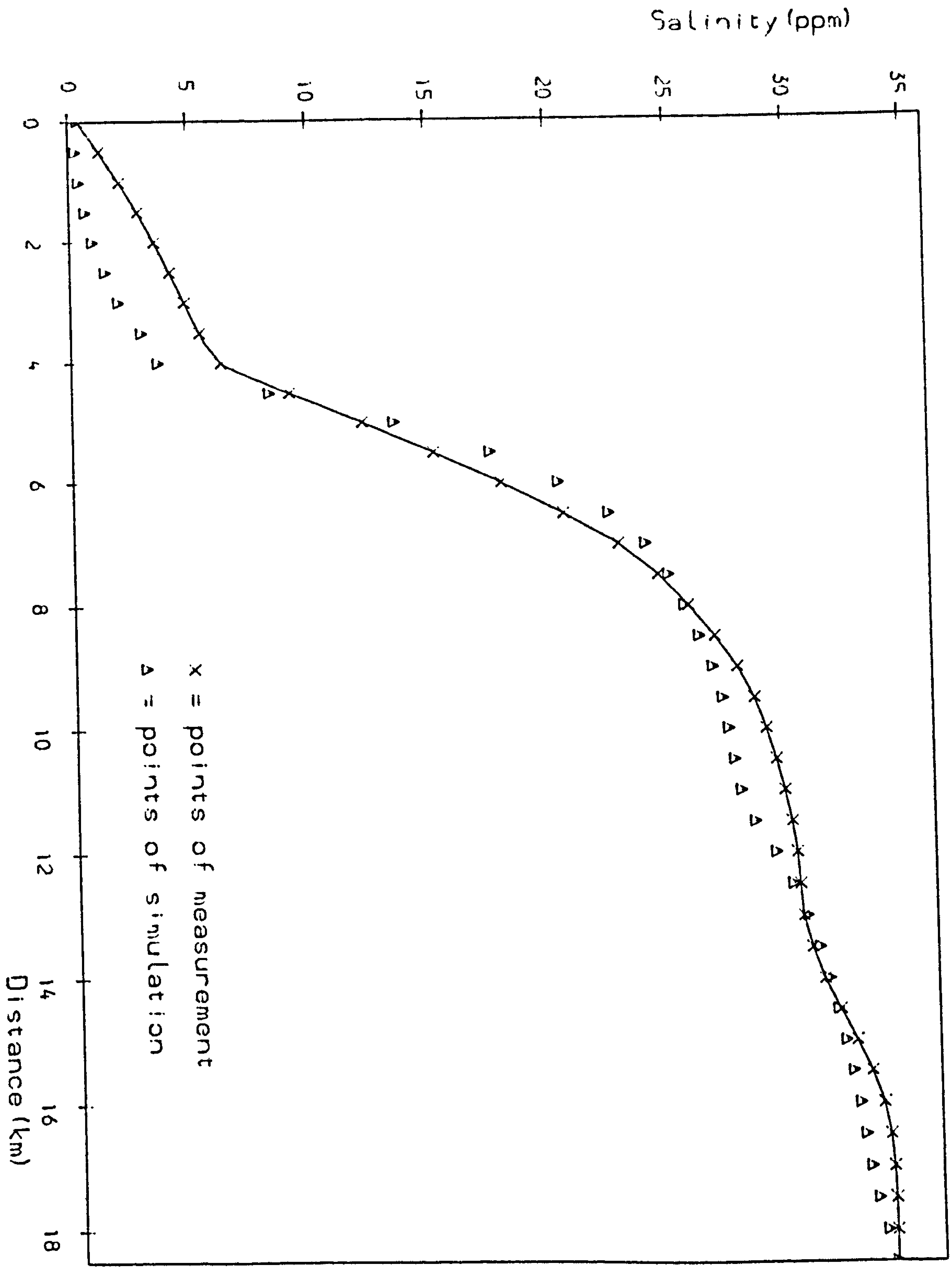

Fig. 7.15 Comparison between measurements and simulations

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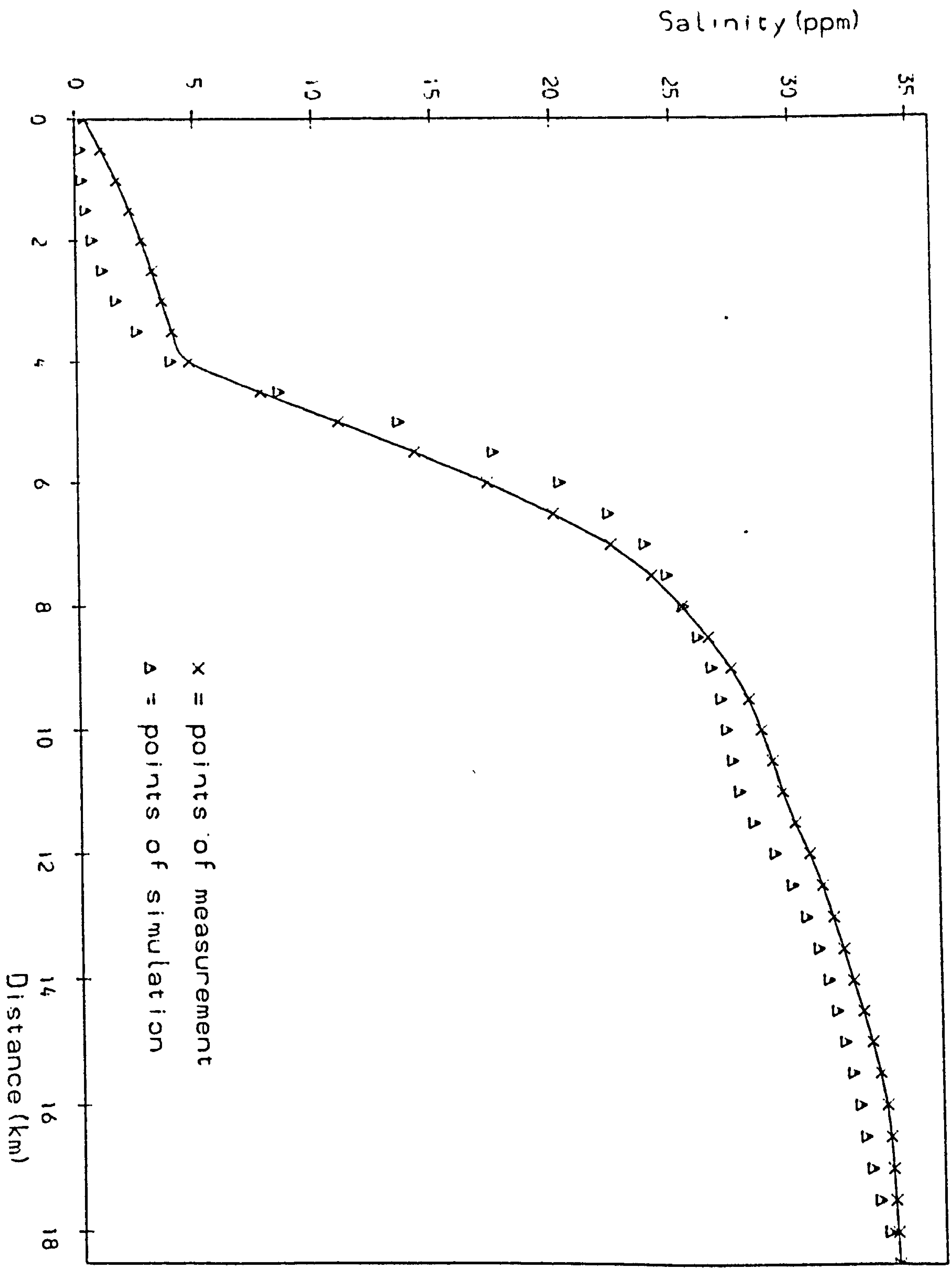

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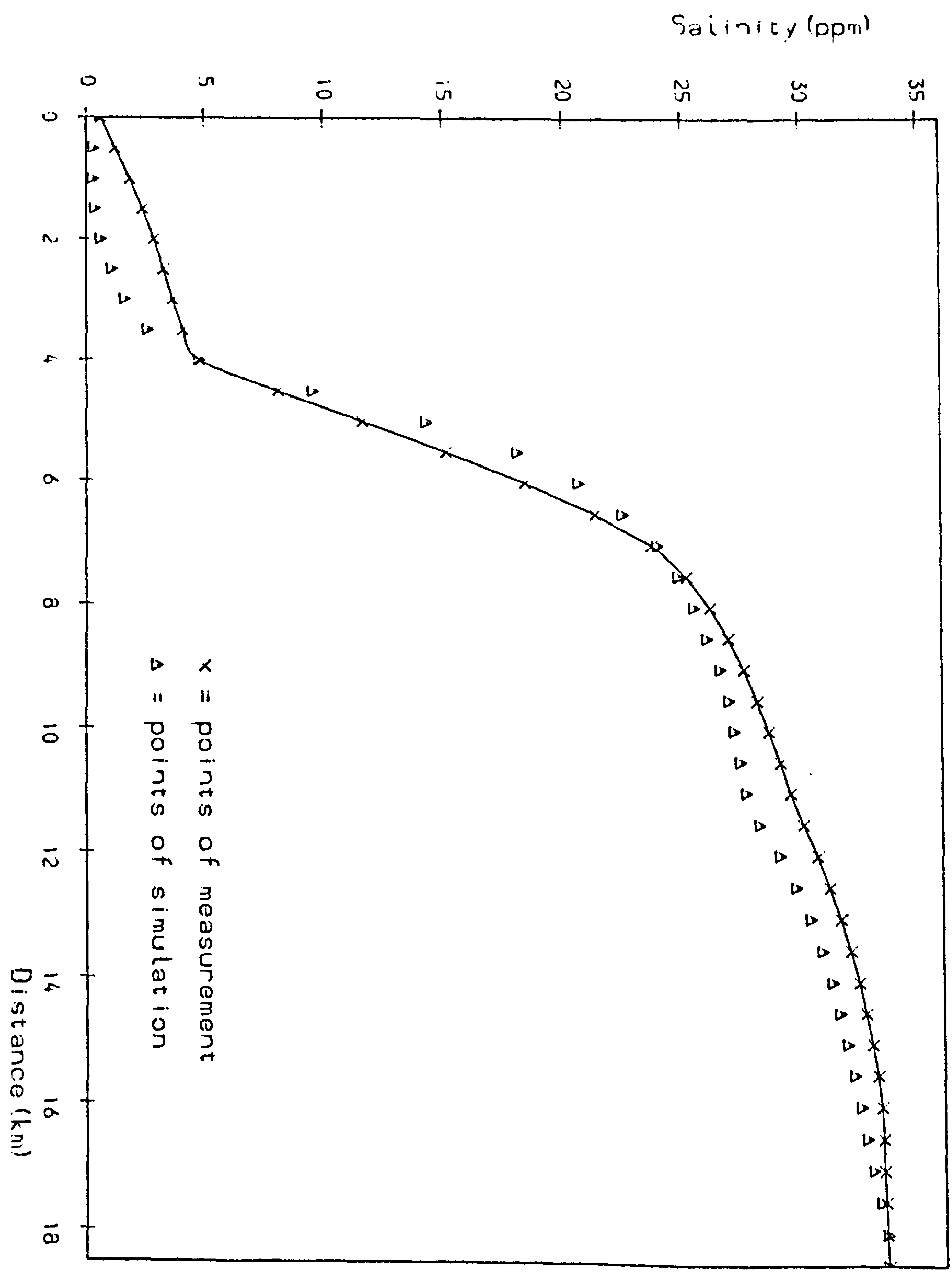

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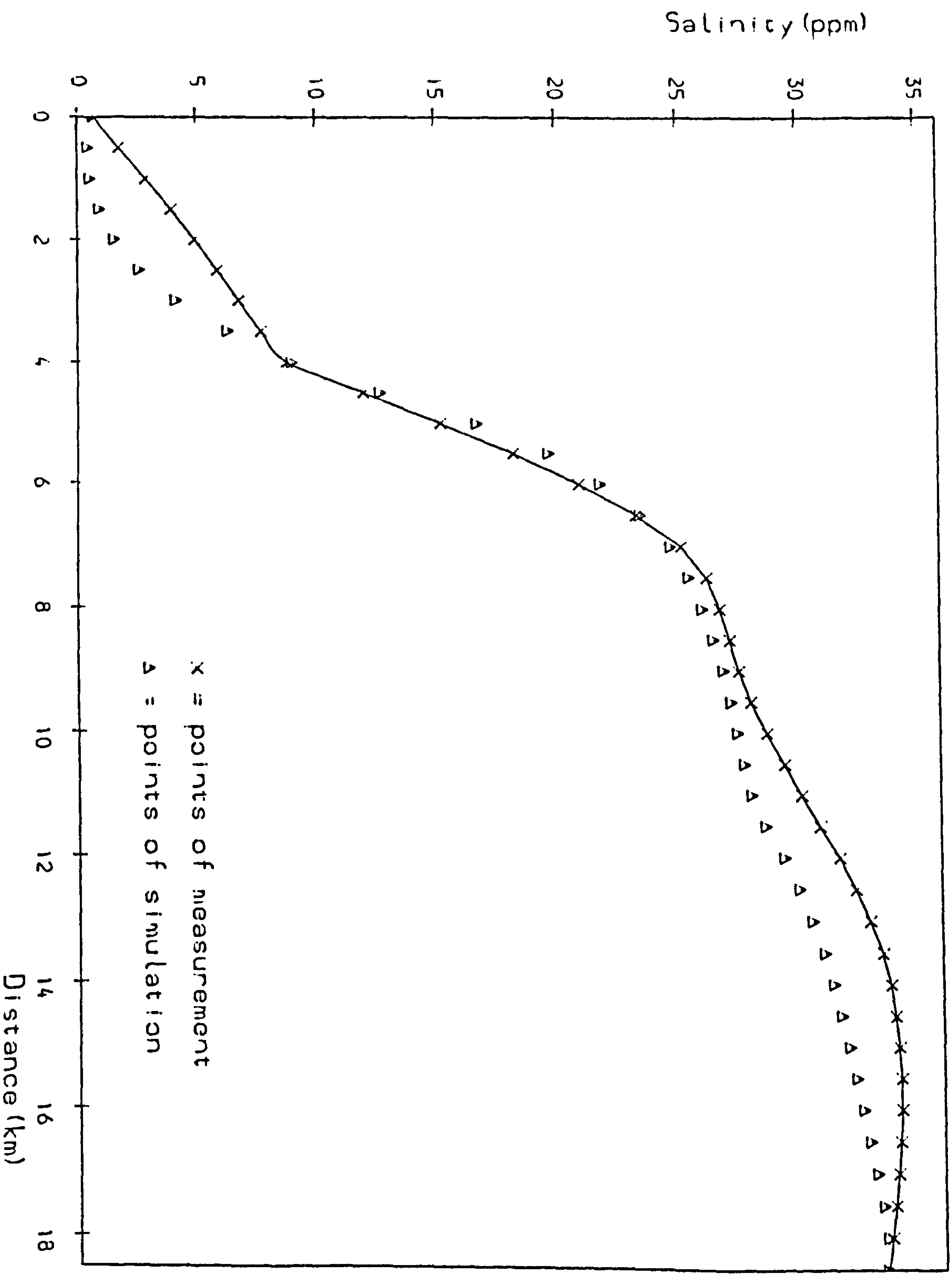

Fig. 7.18 Comparison between measurements and simulations

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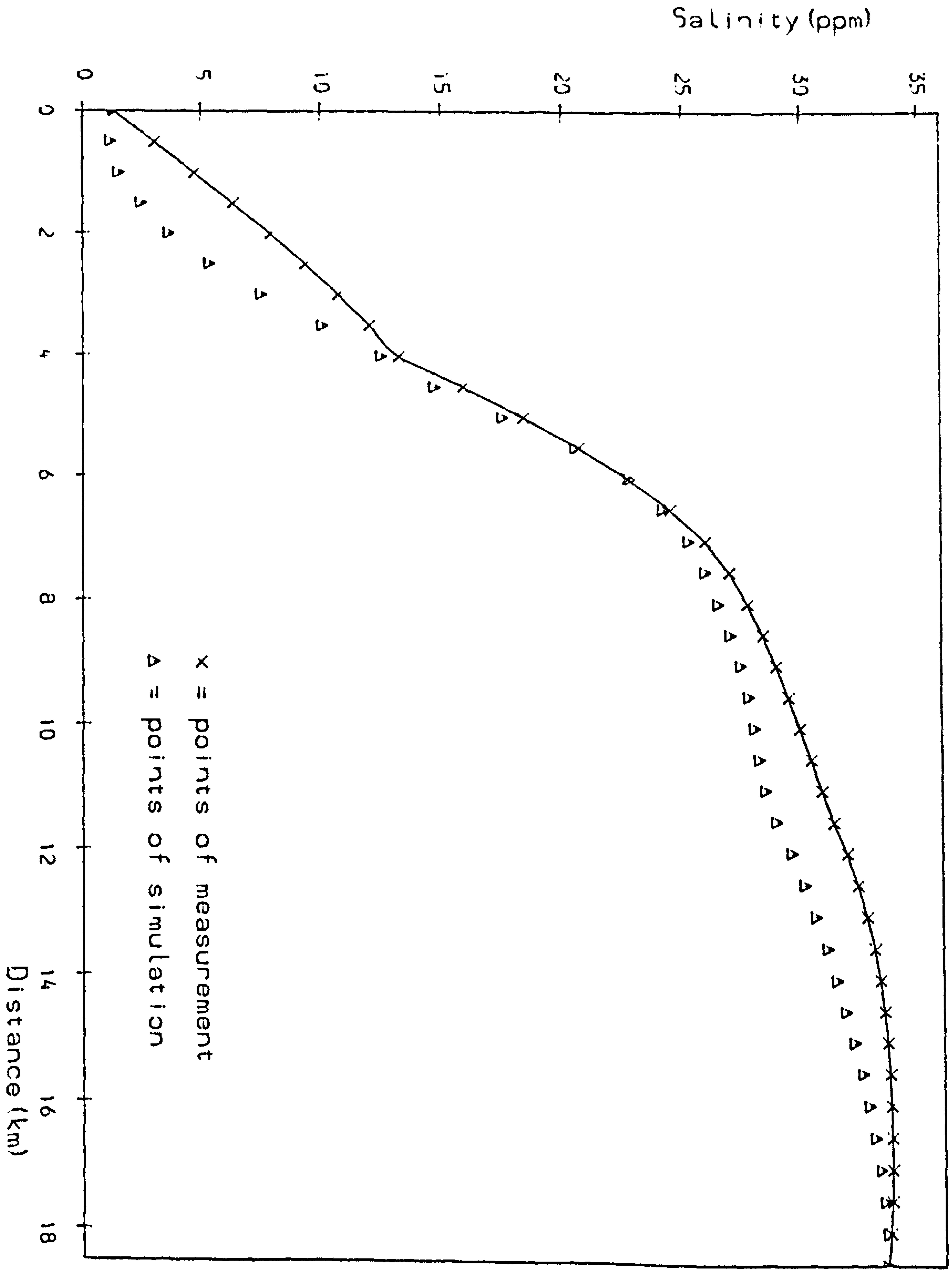

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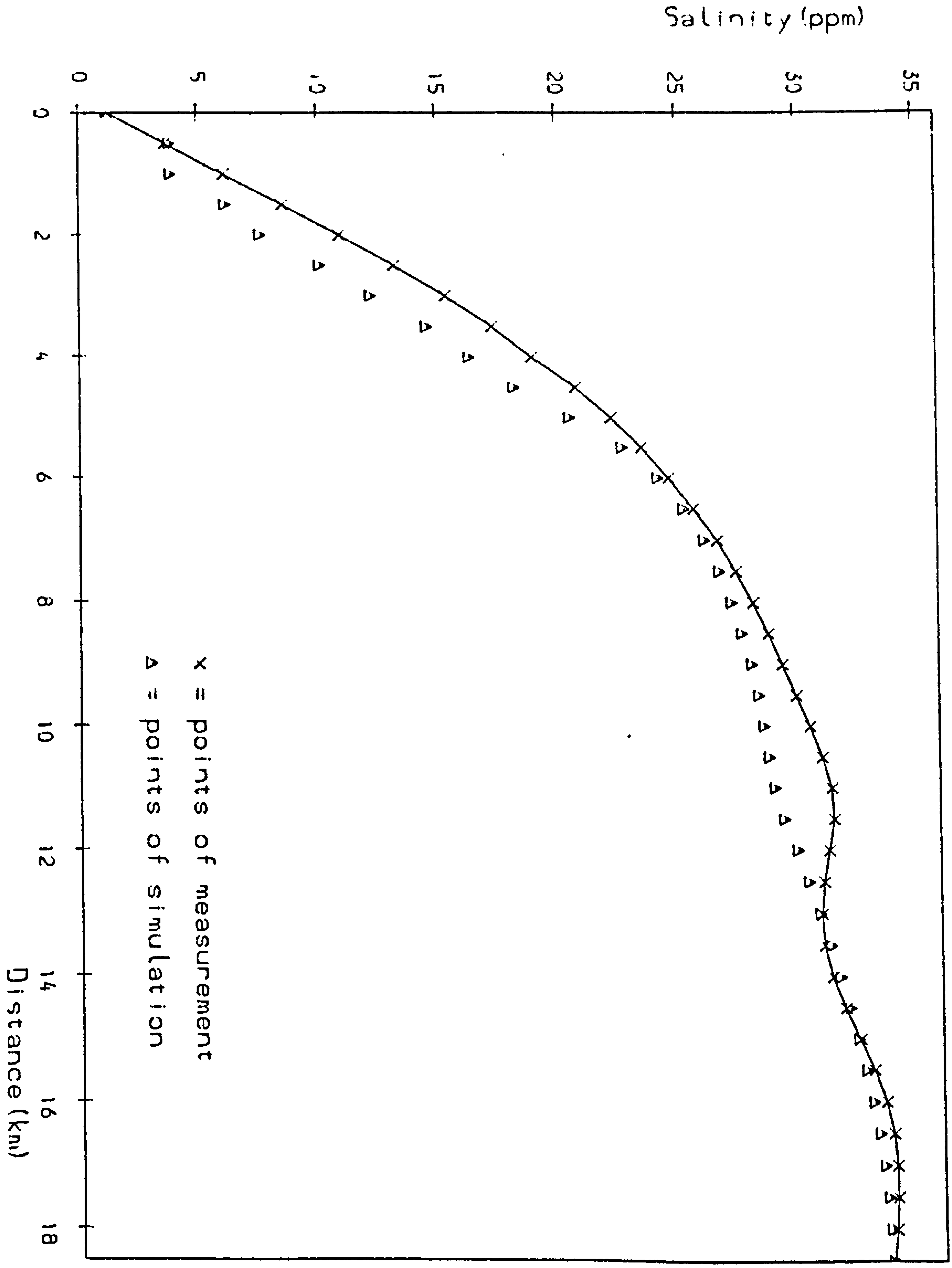

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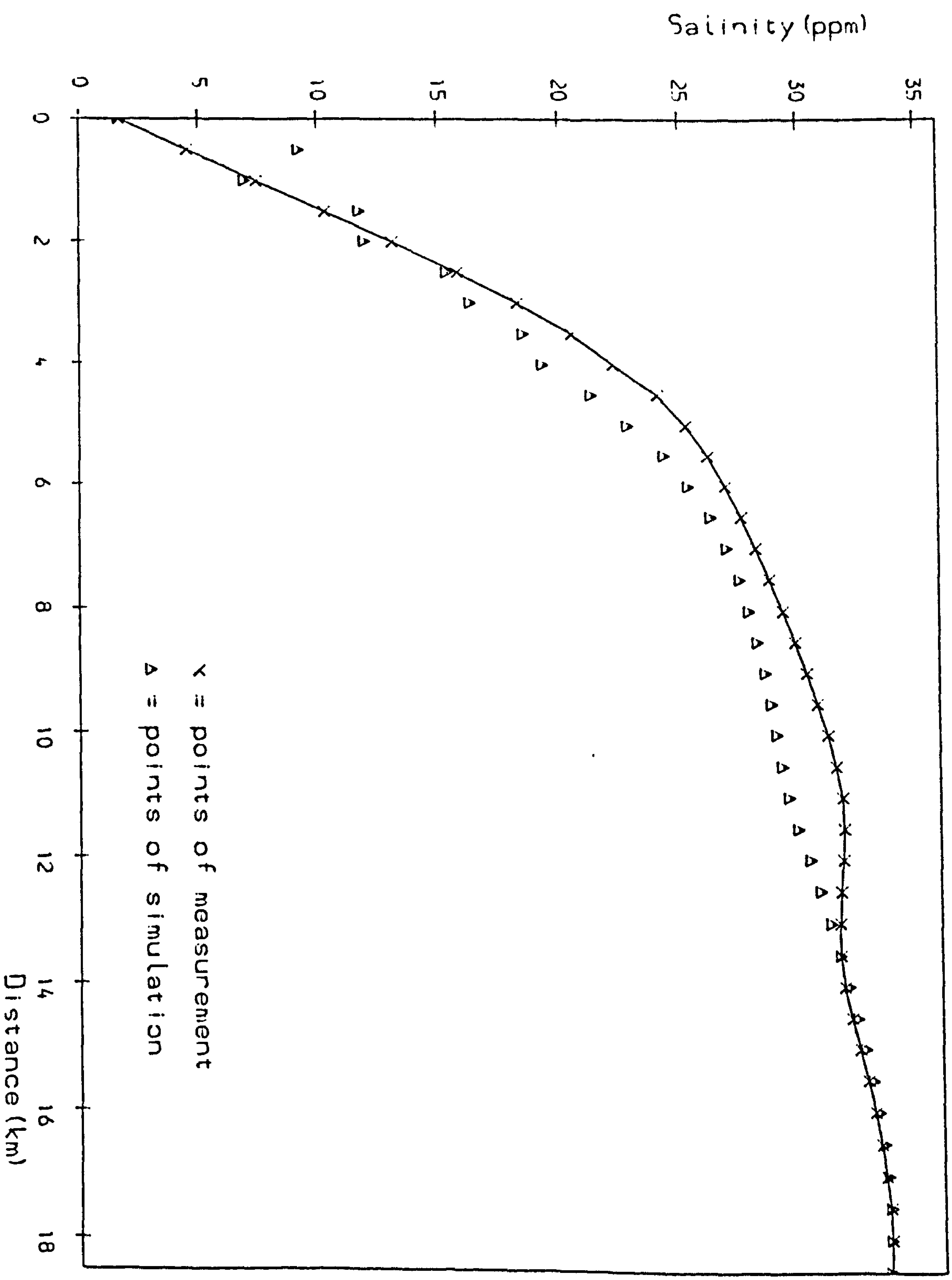

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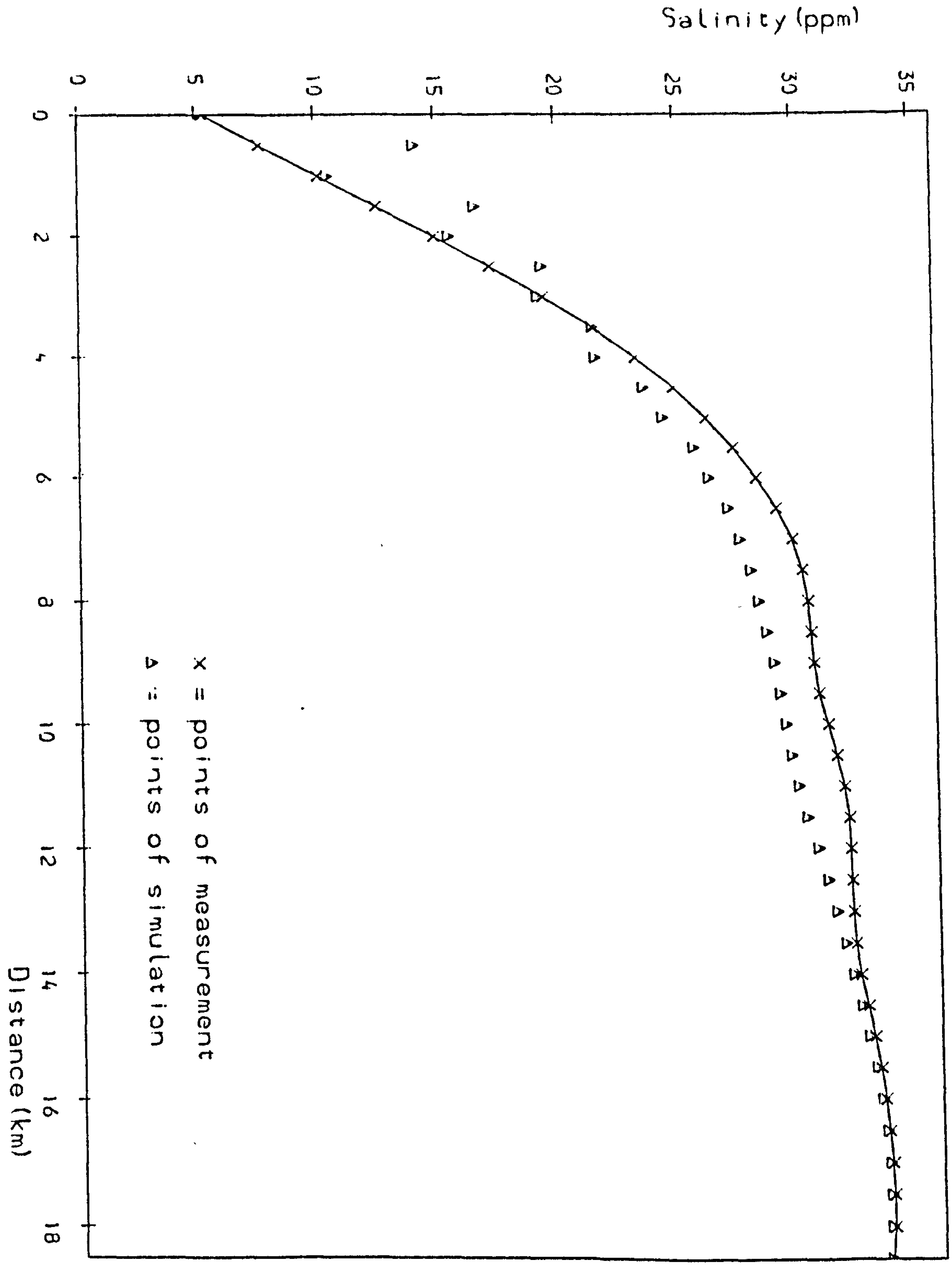

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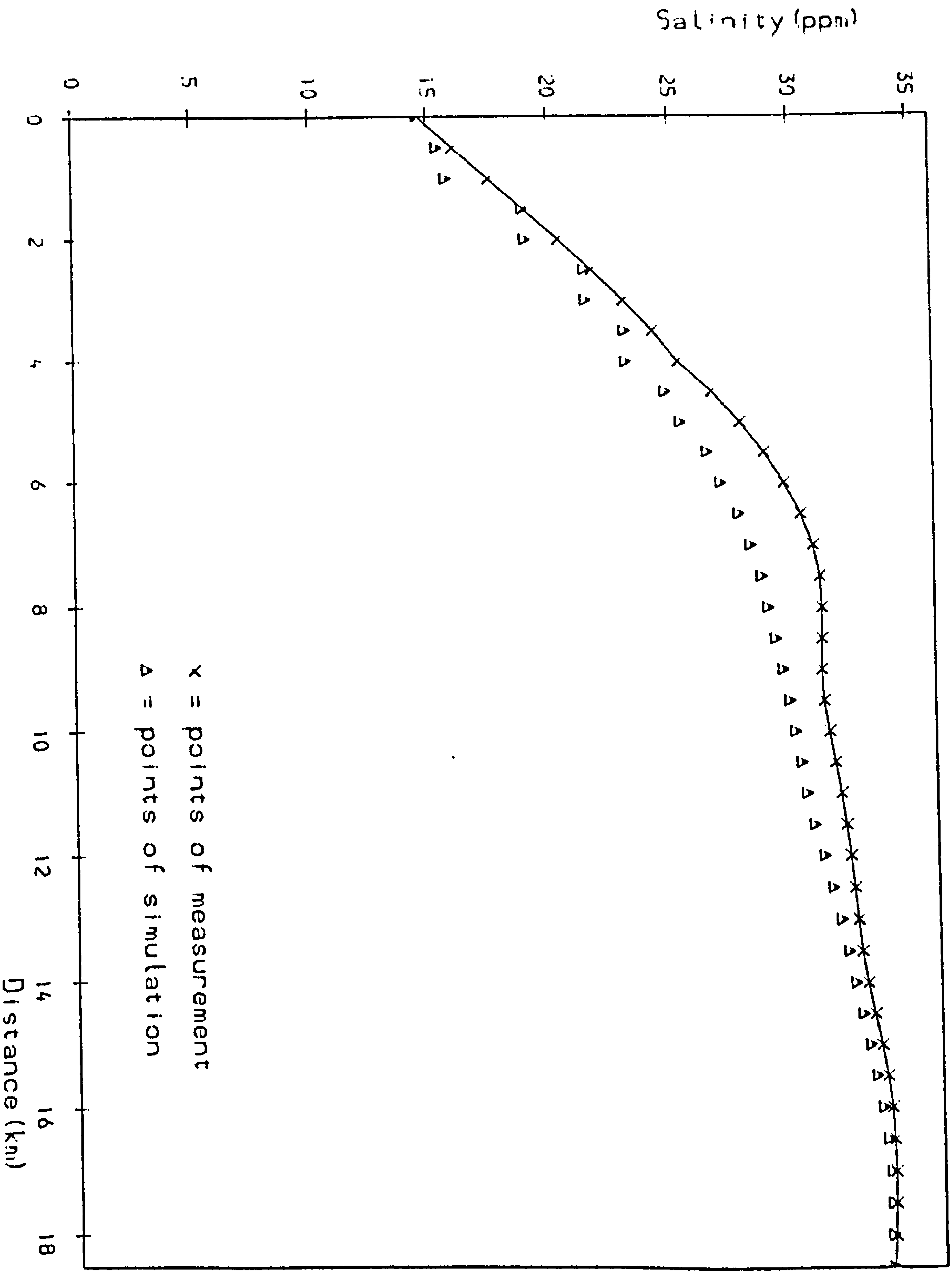

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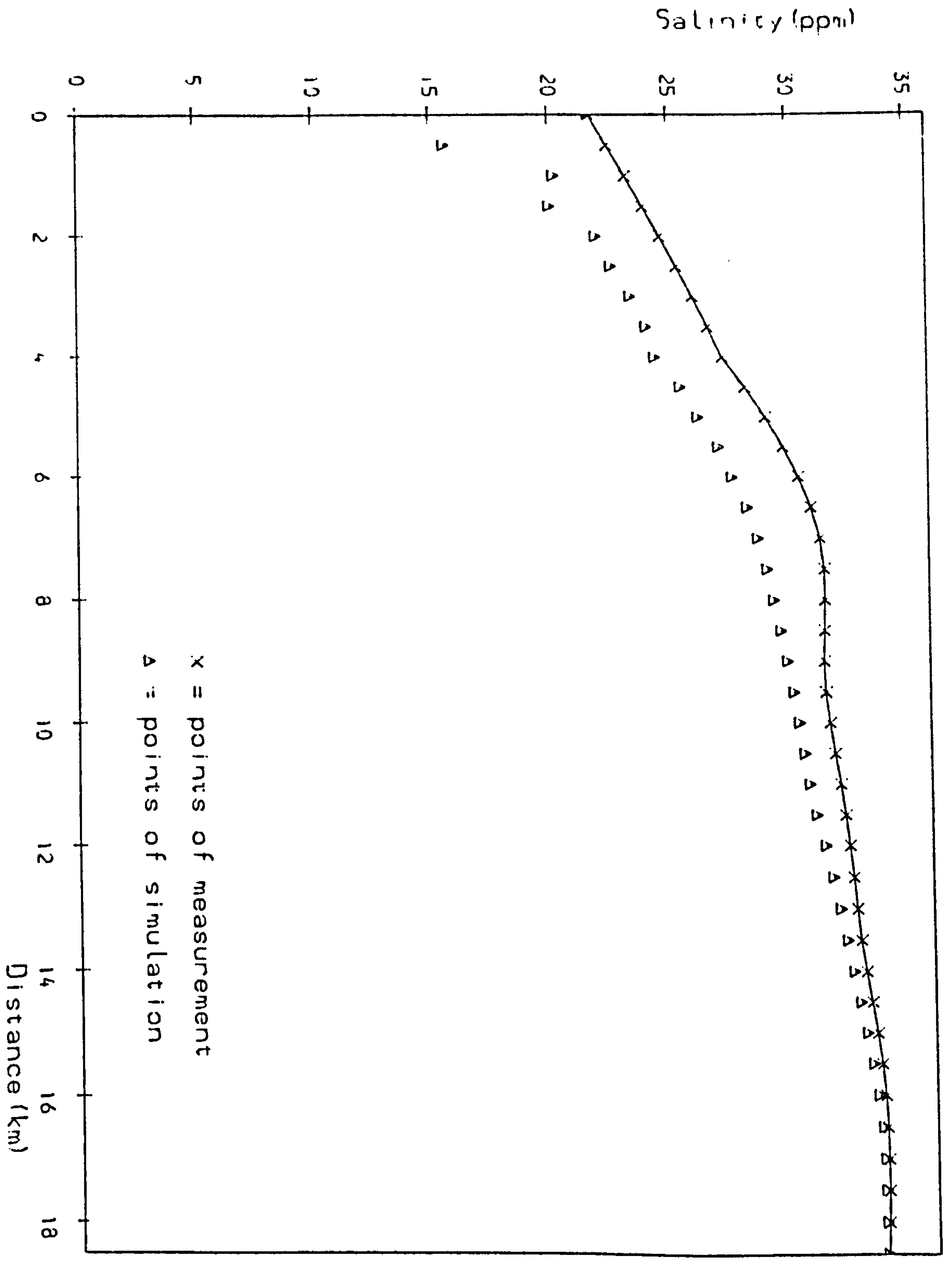

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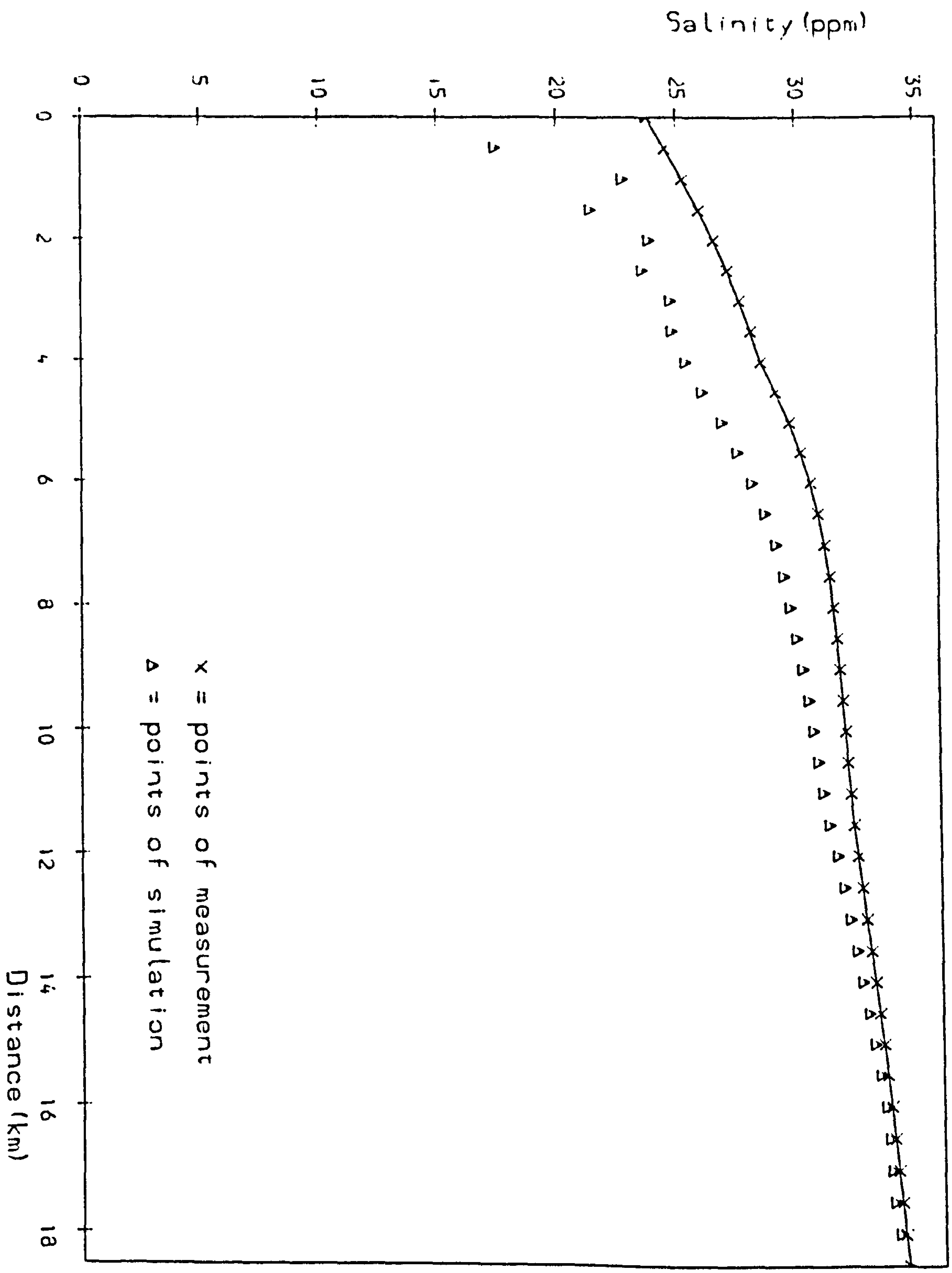

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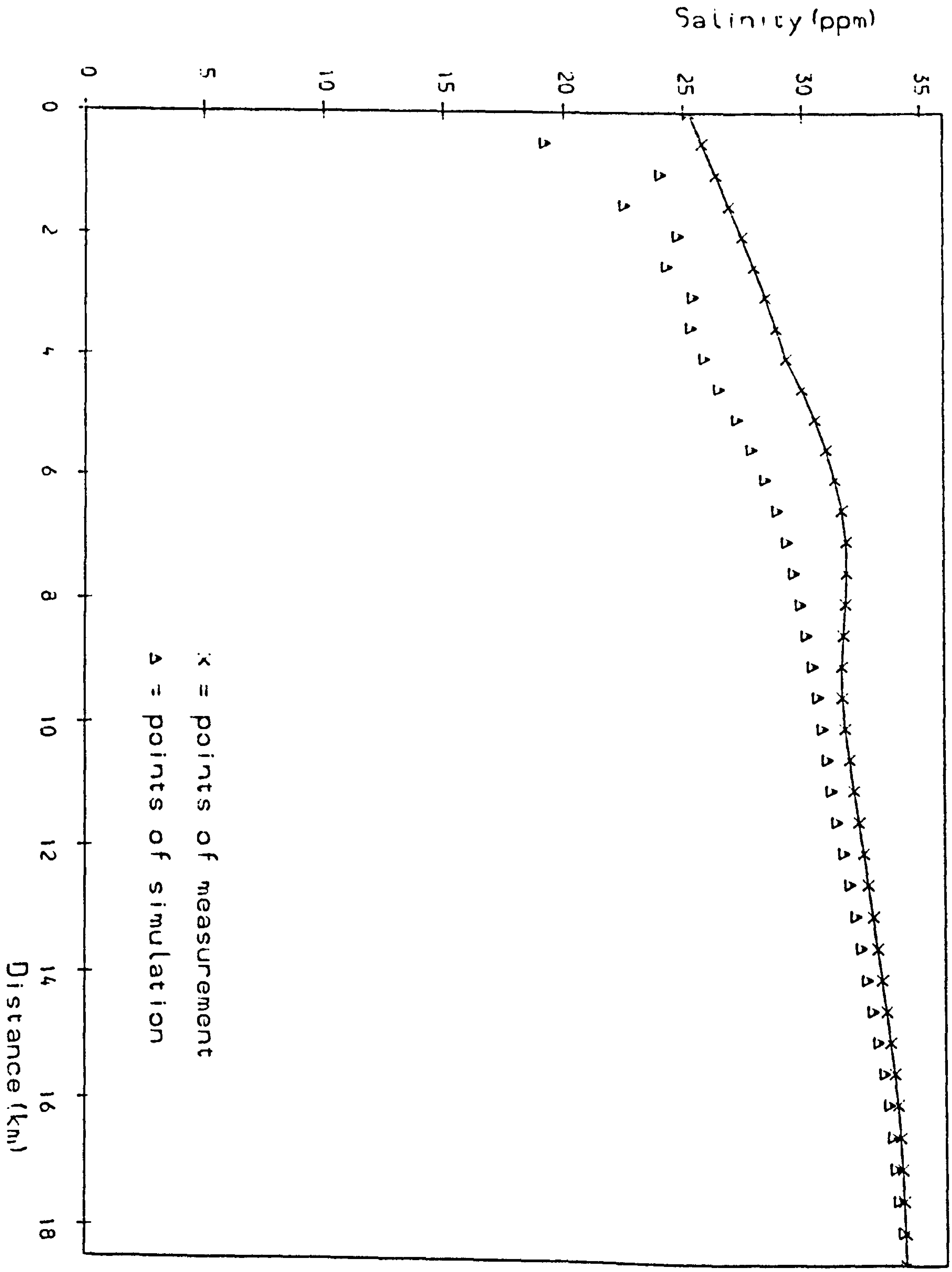

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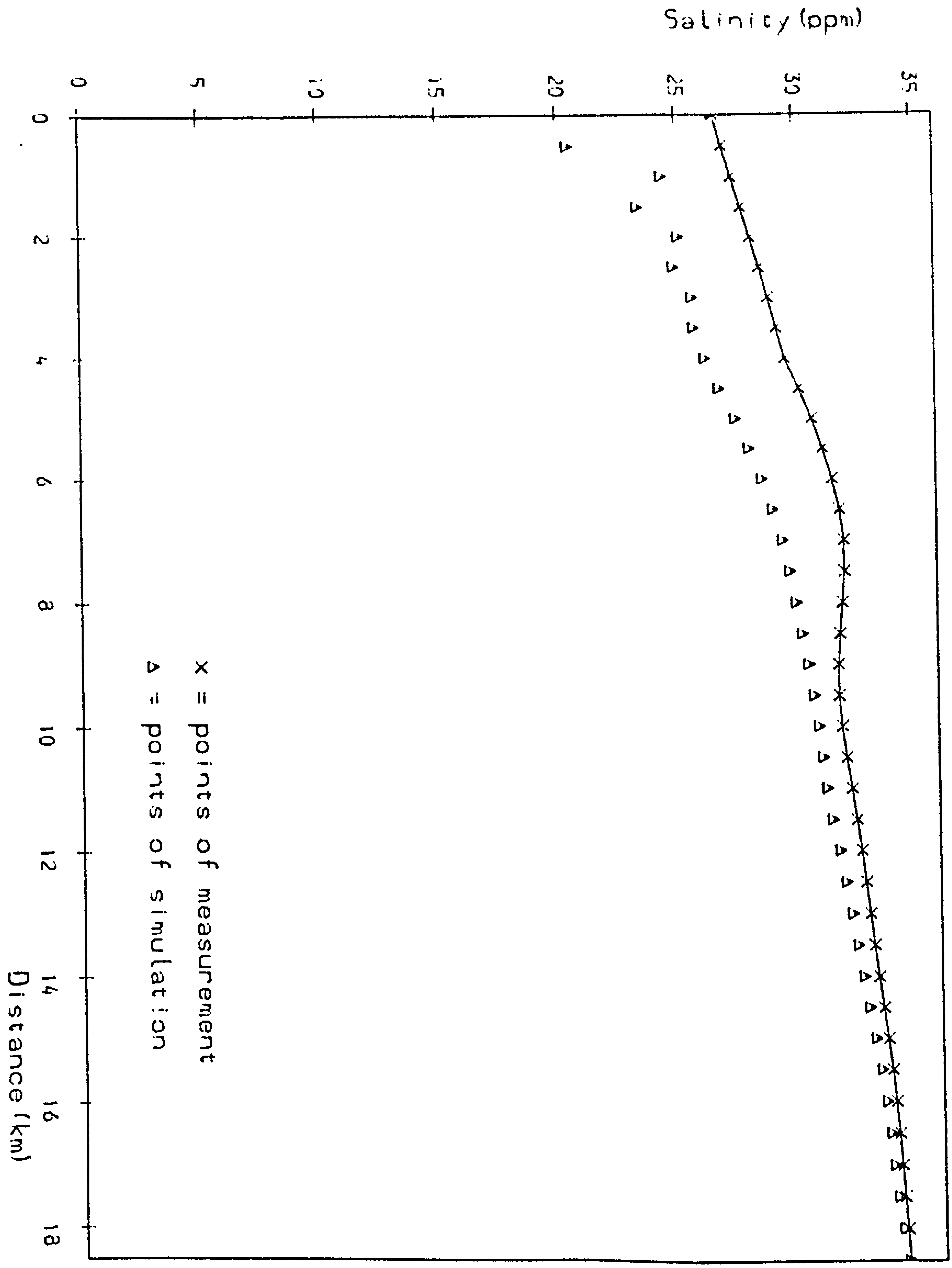


Fig. 7.27 Comparison between measurements and simulations

time=19:00

Fig. 7.28 Comparison between measurements and simulations

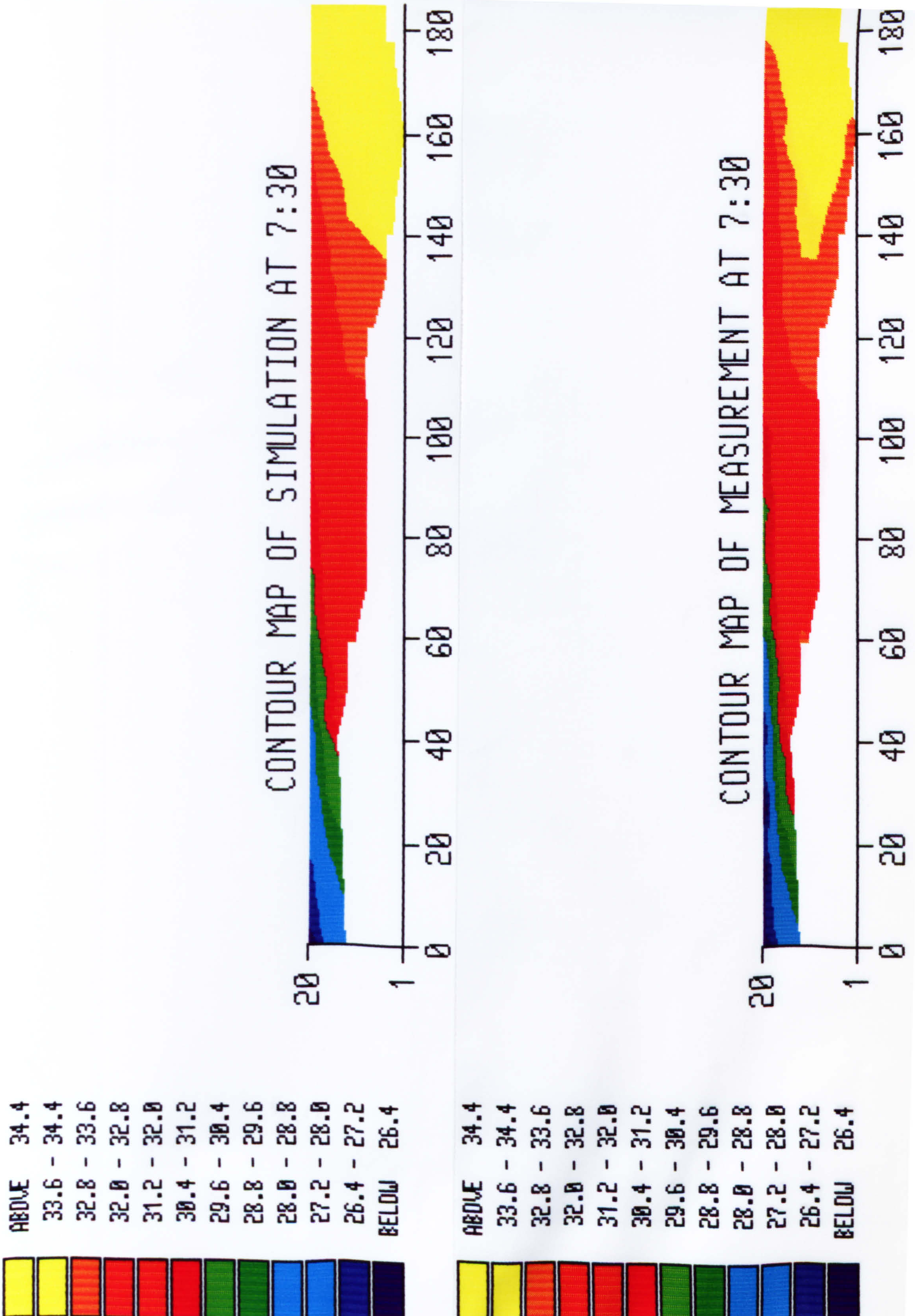


Fig. 7.29 Comparison between measurements and simulations

Fig. 7.30 Comparison between measurements and simulations

Fig. 7.31 Comparison between measurements and simulations

Fig. 7.32 Comparison between measurements and simulations

Fig. 7.33 Comparison between measurements and simulations

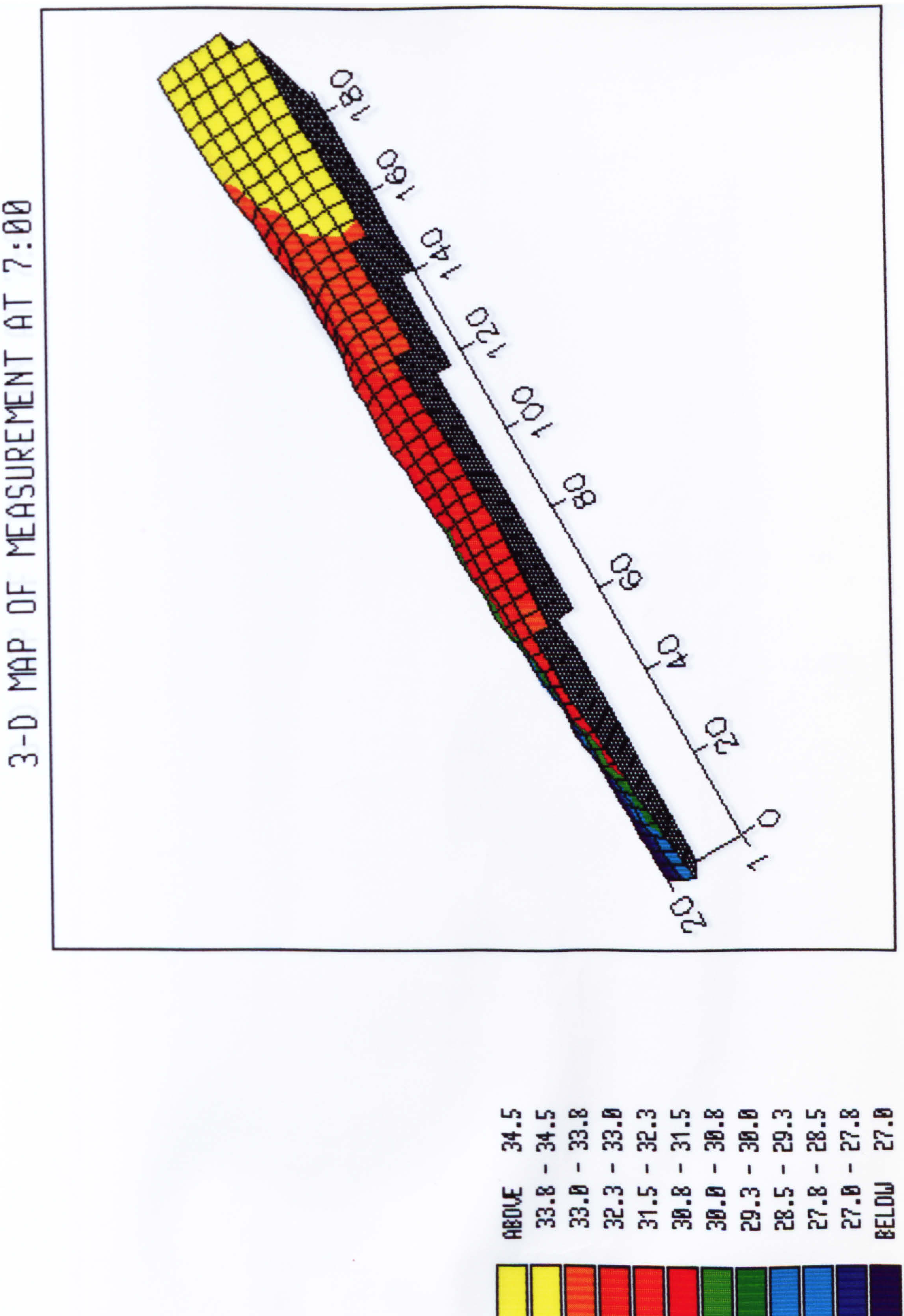


Fig. 7.34 3-D Contour Map

Fig. 7.35 3-D Contour Map

Fig. 7.36 3-D Contour Map

Fig. 7.37 3-D Contour Map

Fig. 7.38 3-D Contour Map

Fig. 7.39 3-D Contour Map

Fig. 7.40 3-D Contour Map

Fig. 7.41 3-D Contour Map

Fig. 7.42 3-D Contour Map

Fig. 7.43 3-D Contour Map

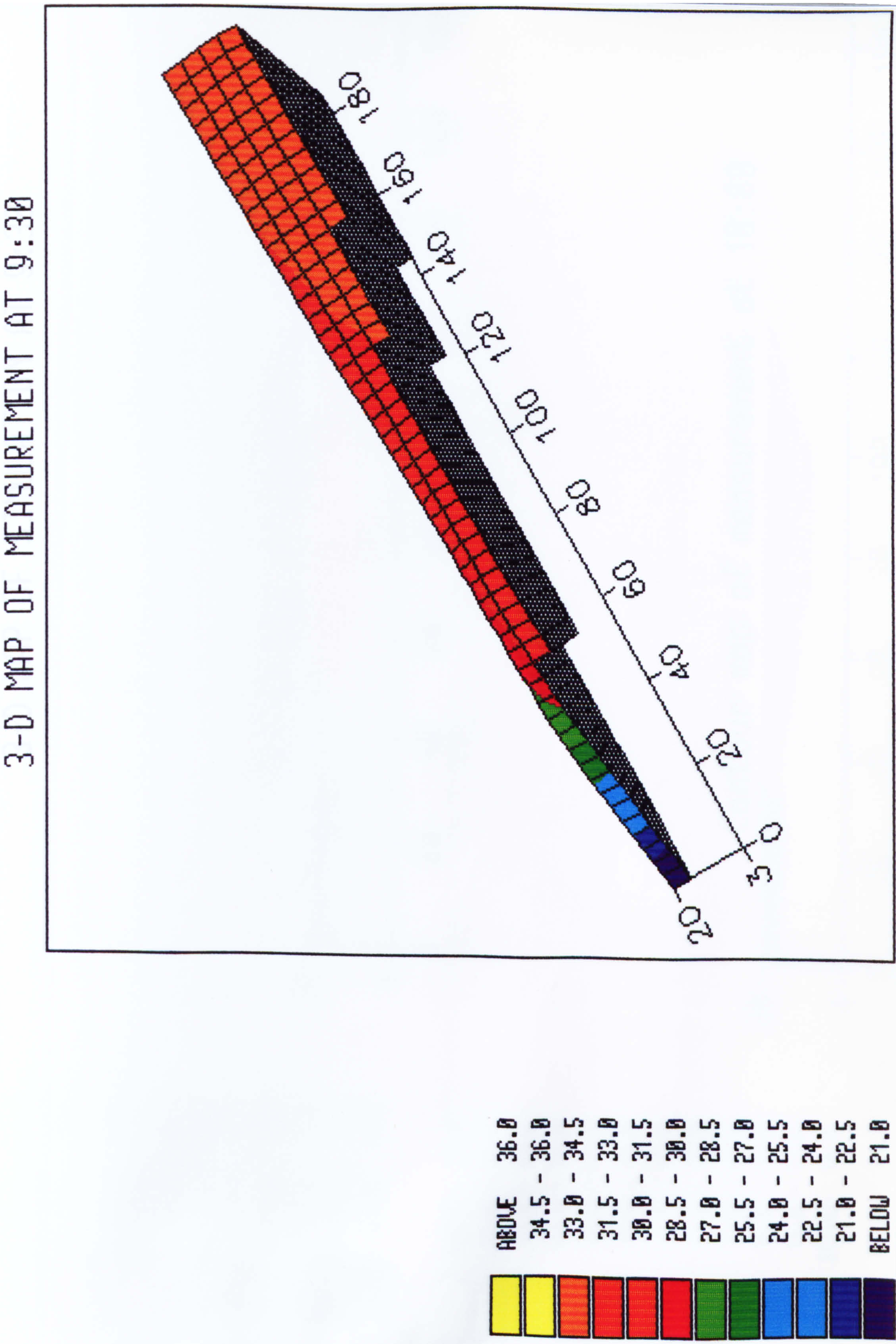


Fig. 7.44 3-D Contour Map

Fig. 7.45 3-D Contour Map

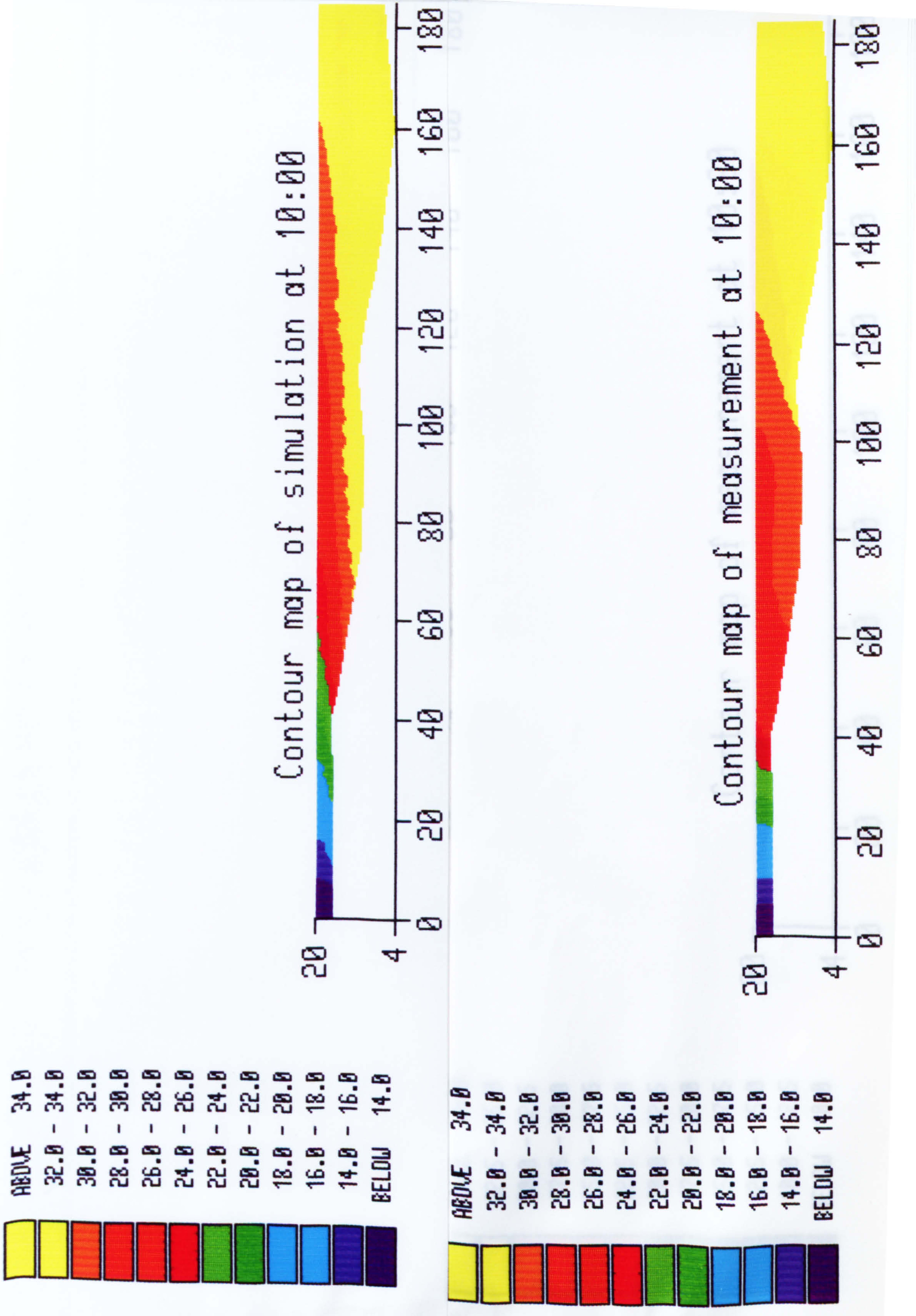
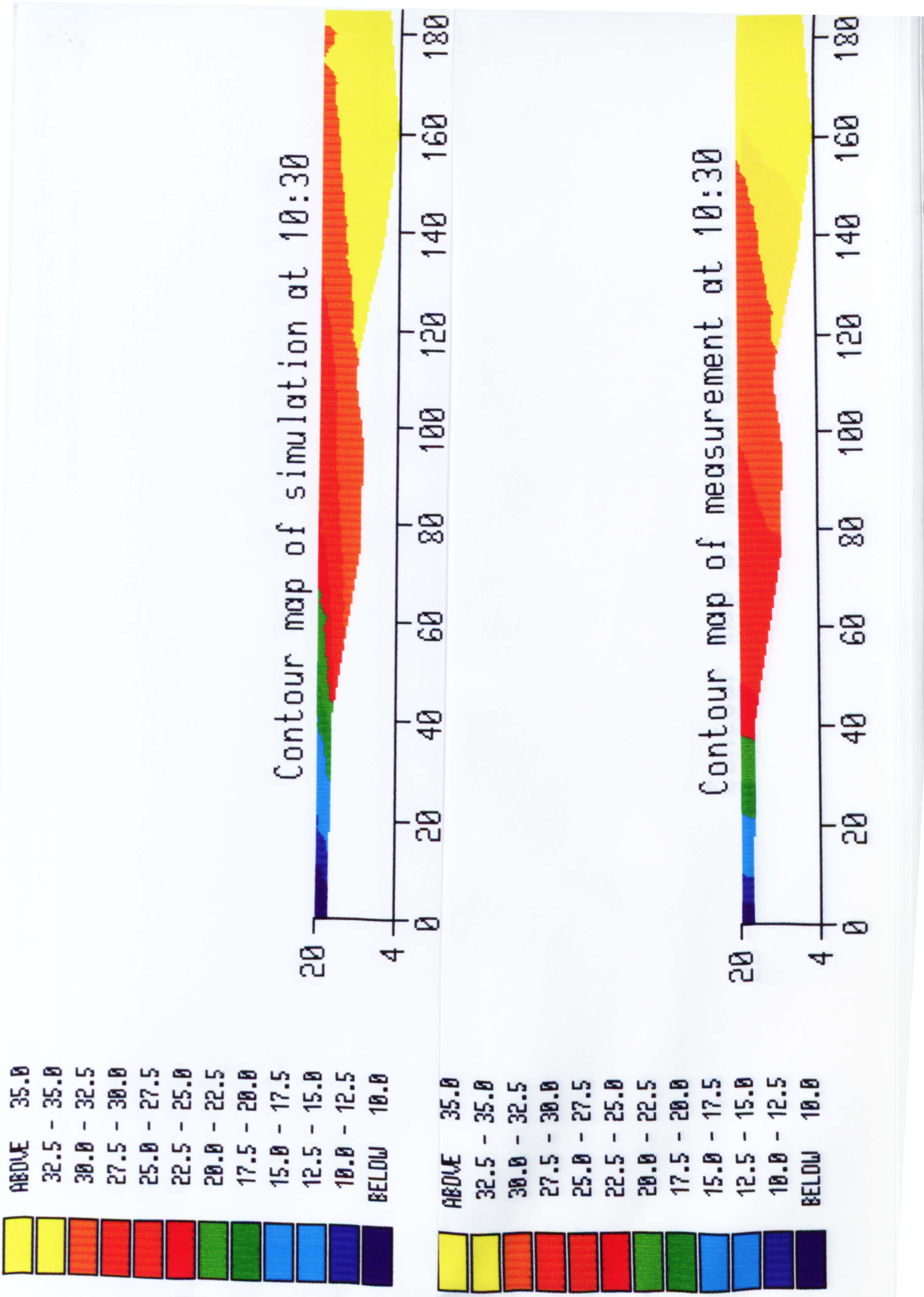


Fig. 7.46 Comparison between measurements and simulations



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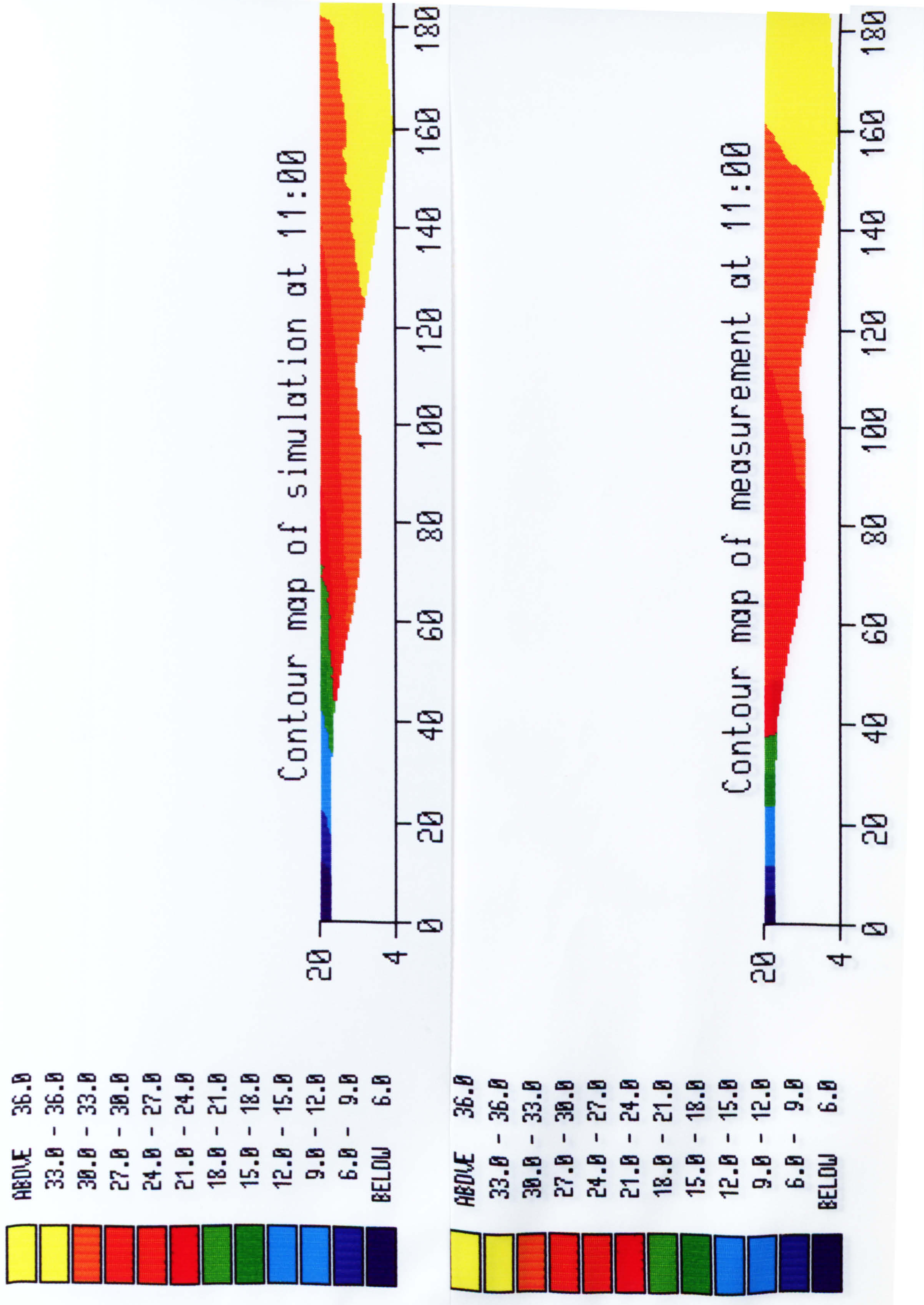

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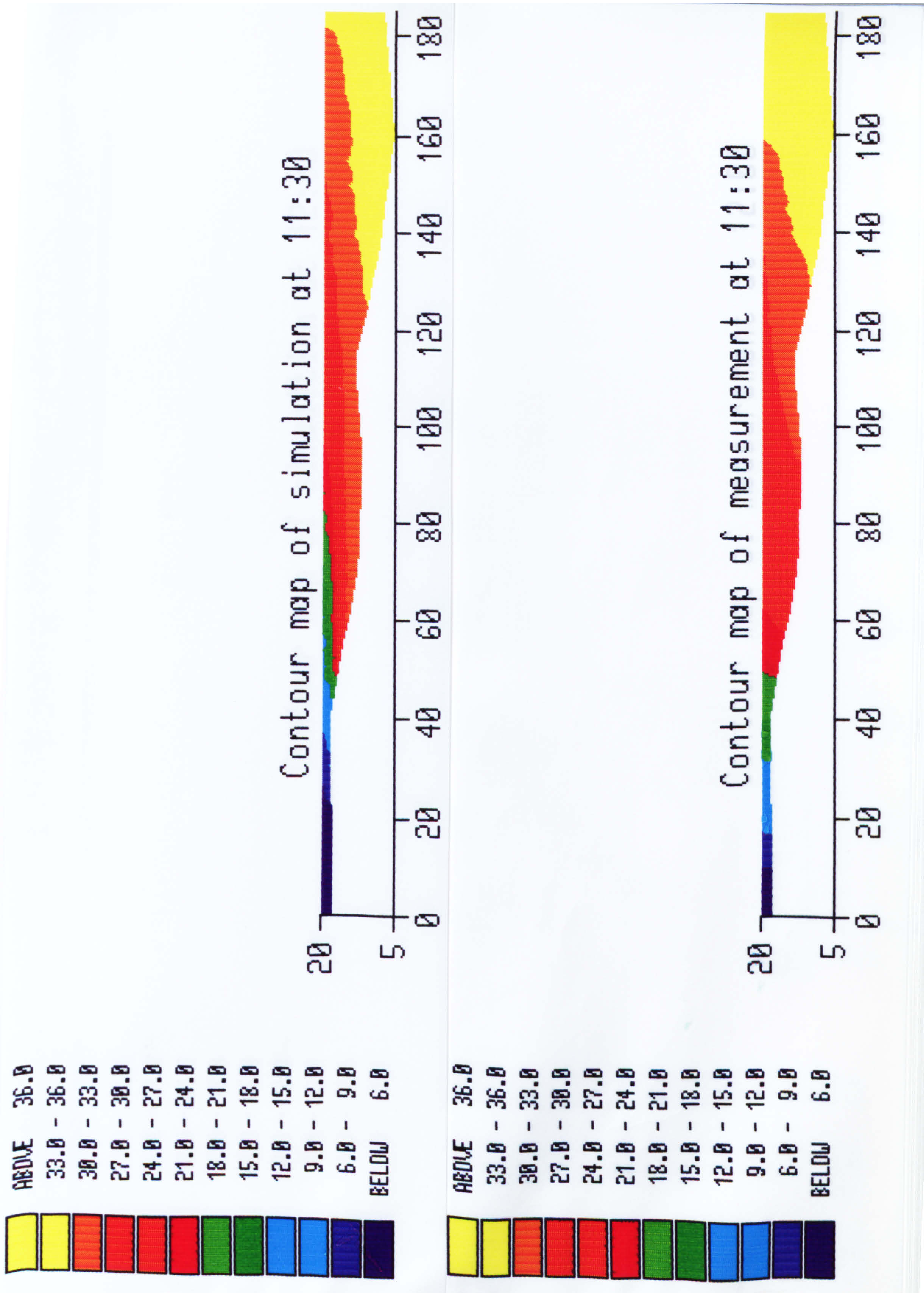

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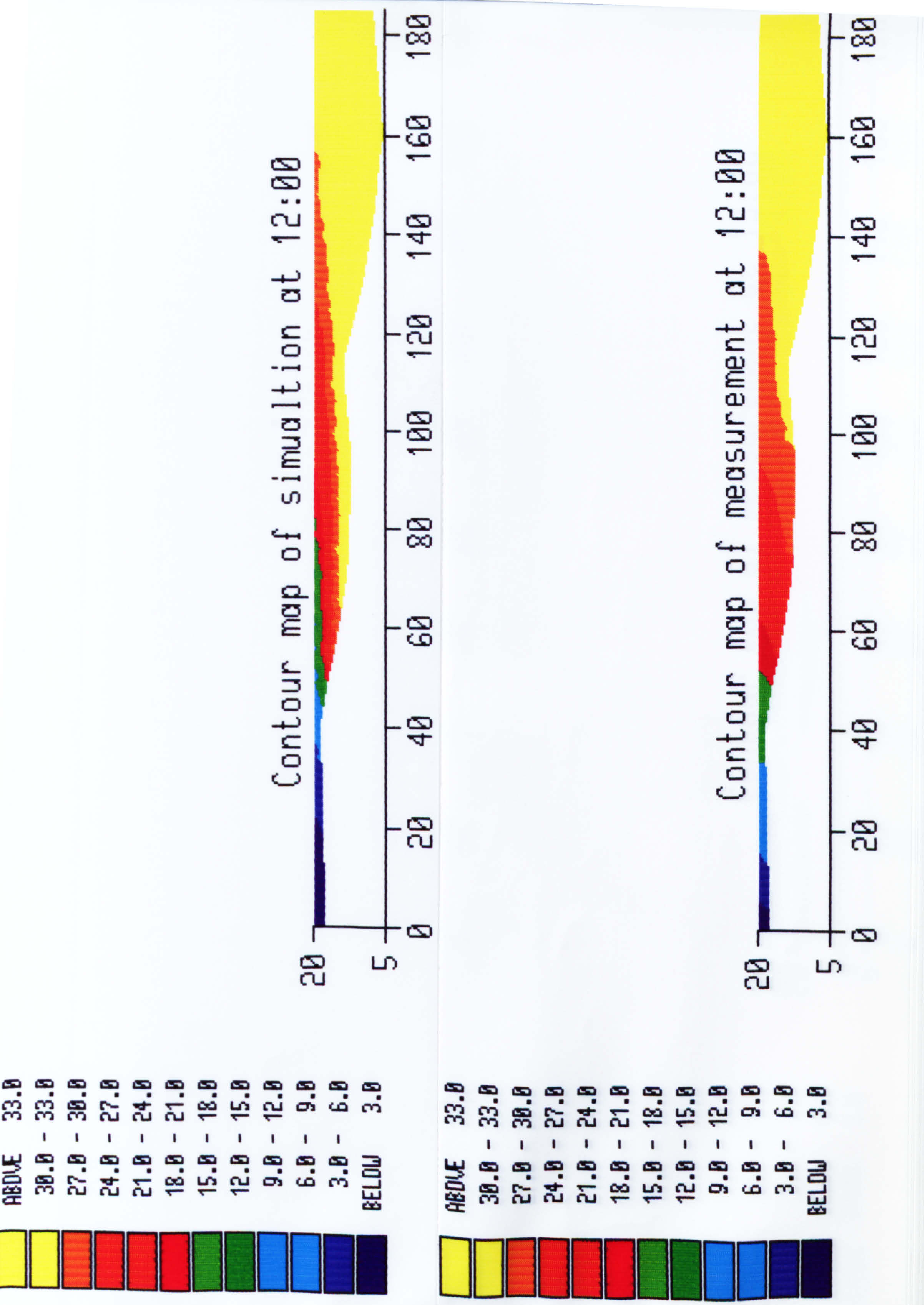

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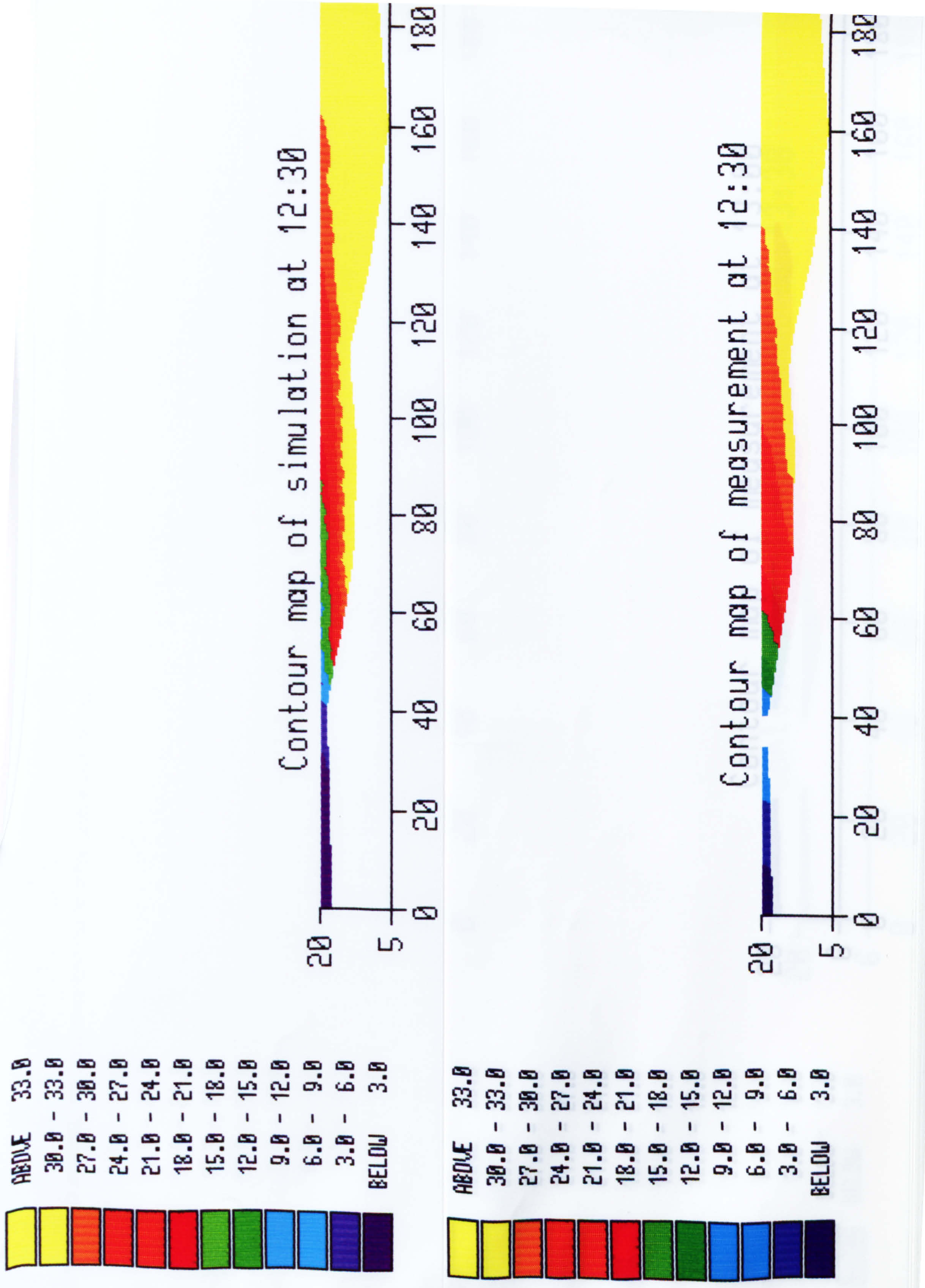

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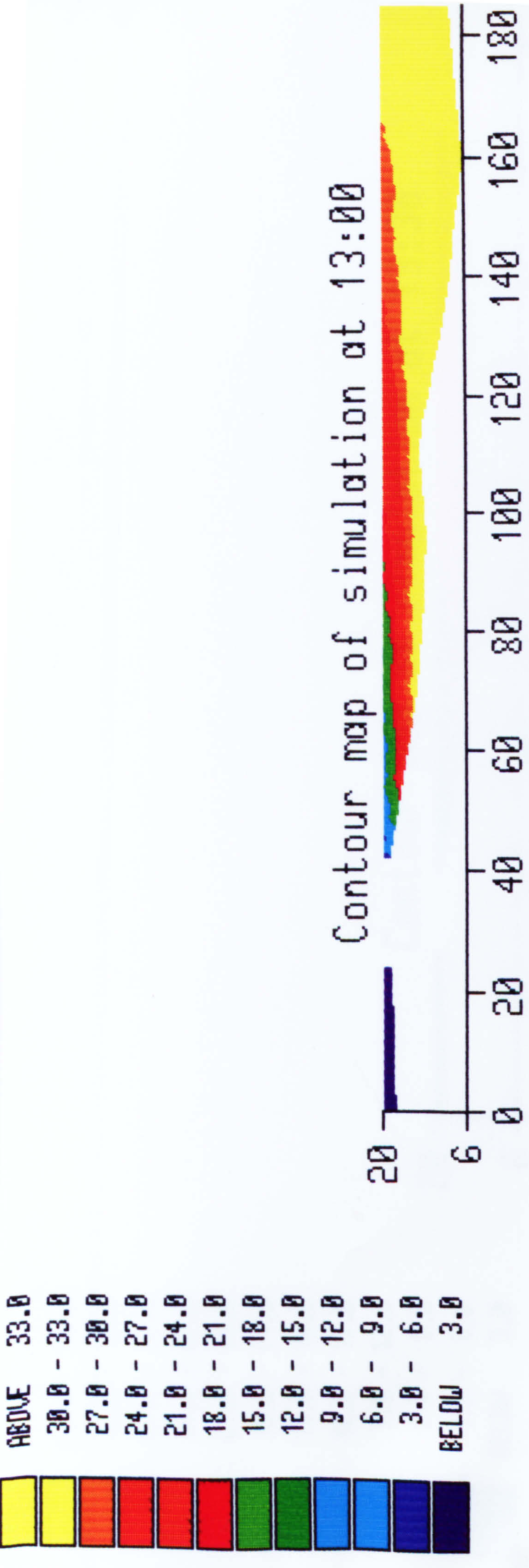


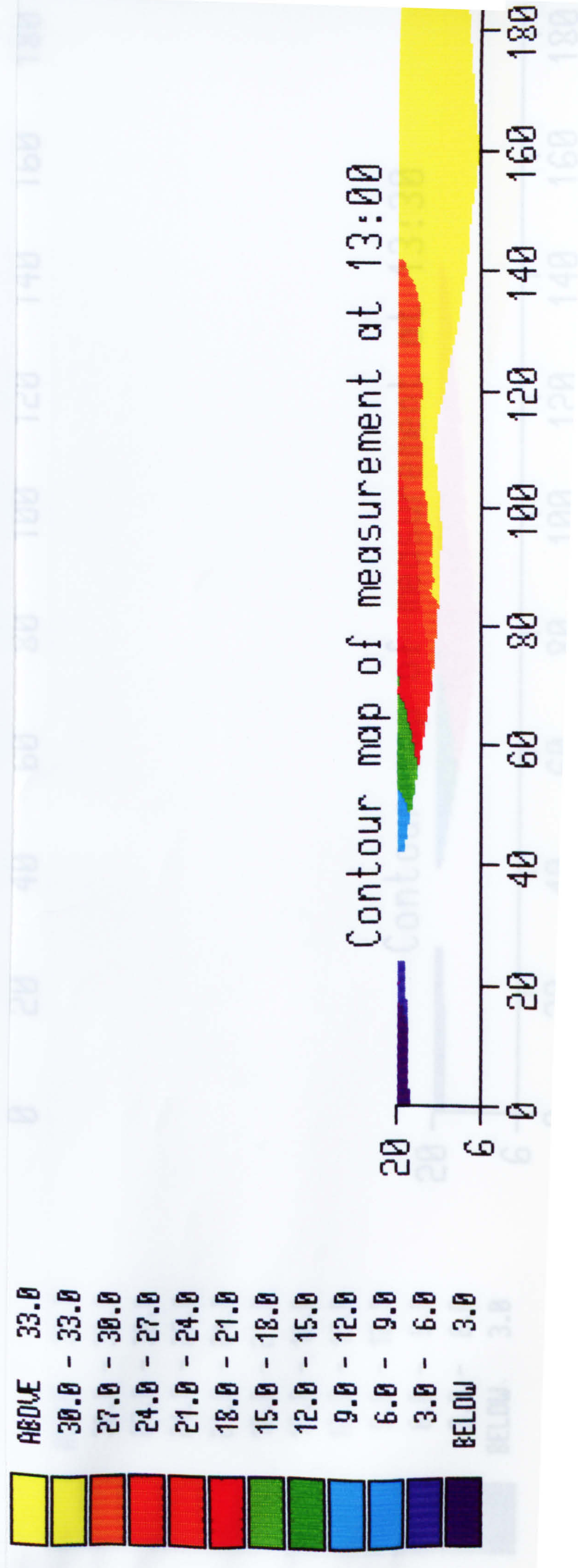
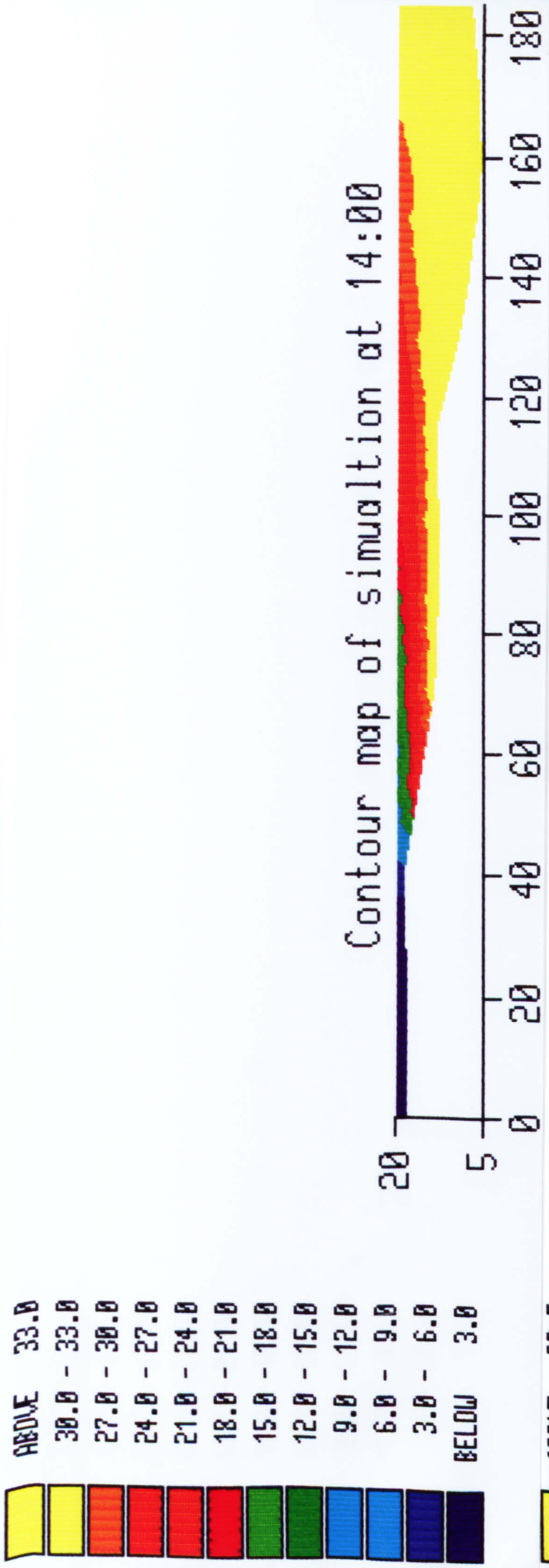
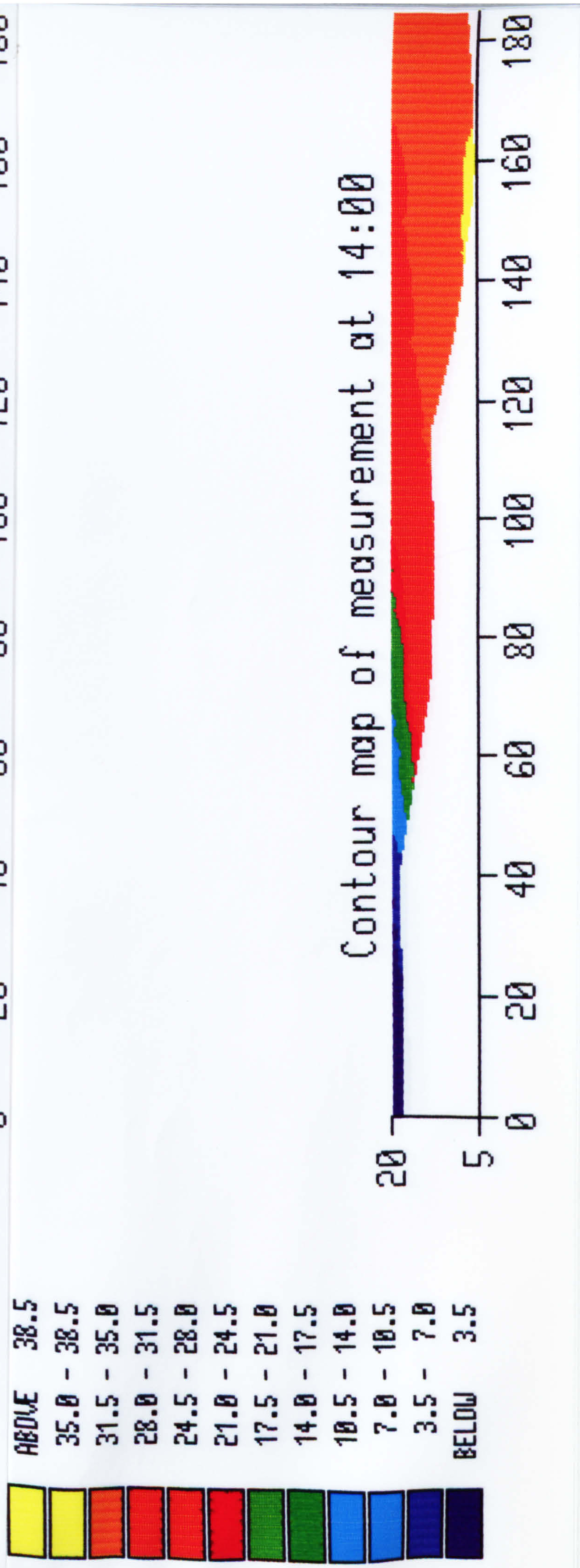


Fig. 7.52 Comparison between measurements and simulations

Fig. 7.53 Comparison between measurements and simulations





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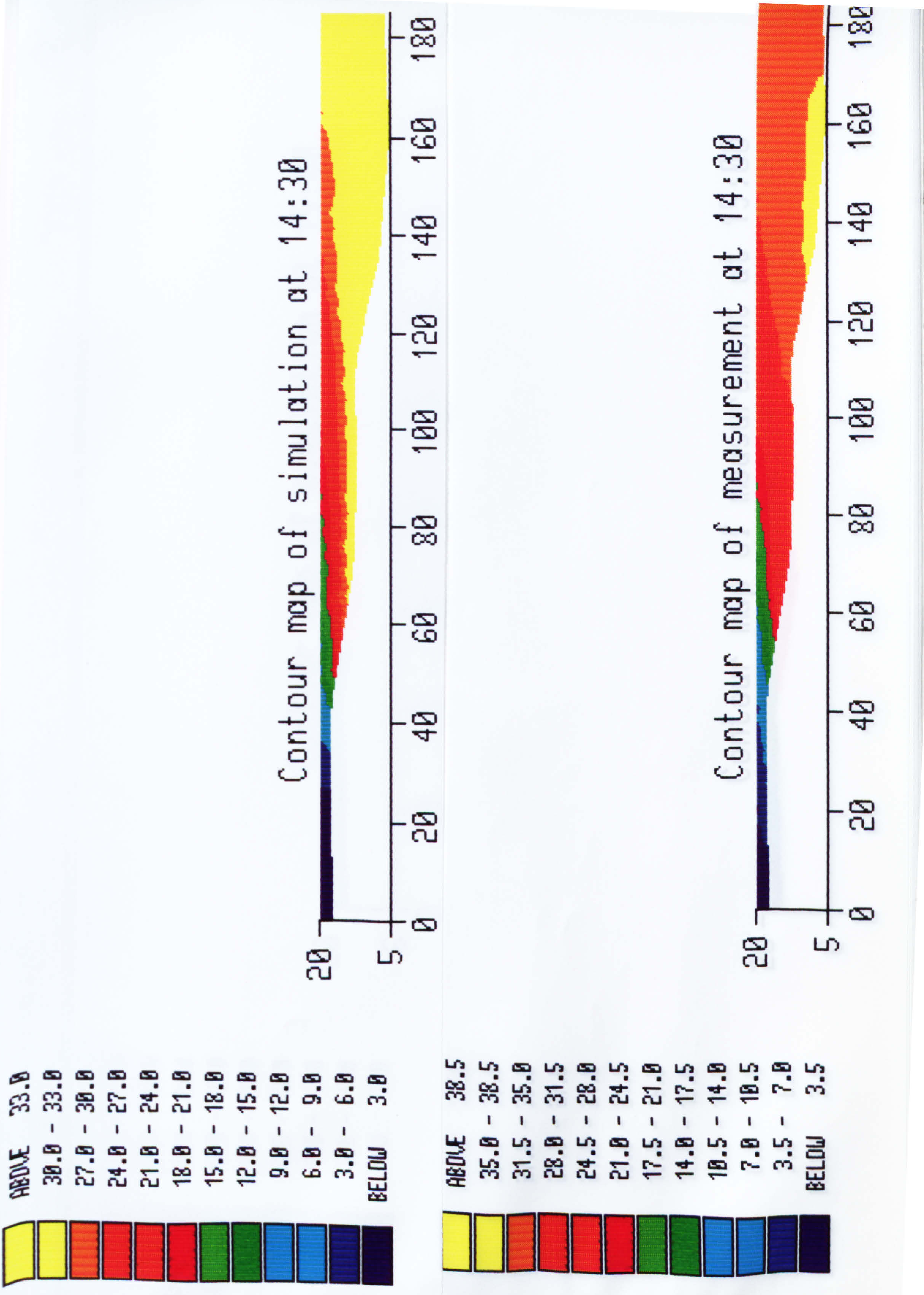

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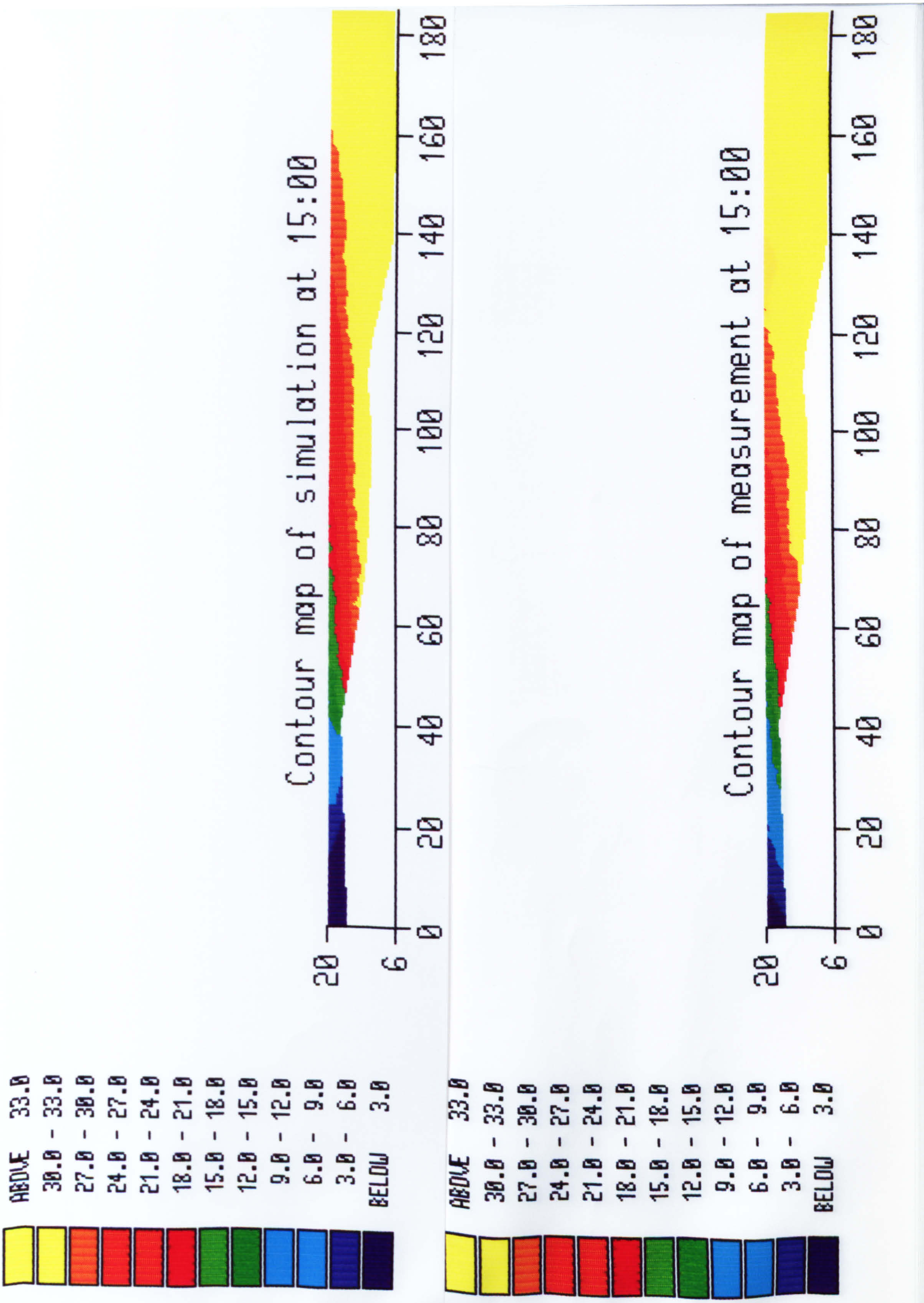

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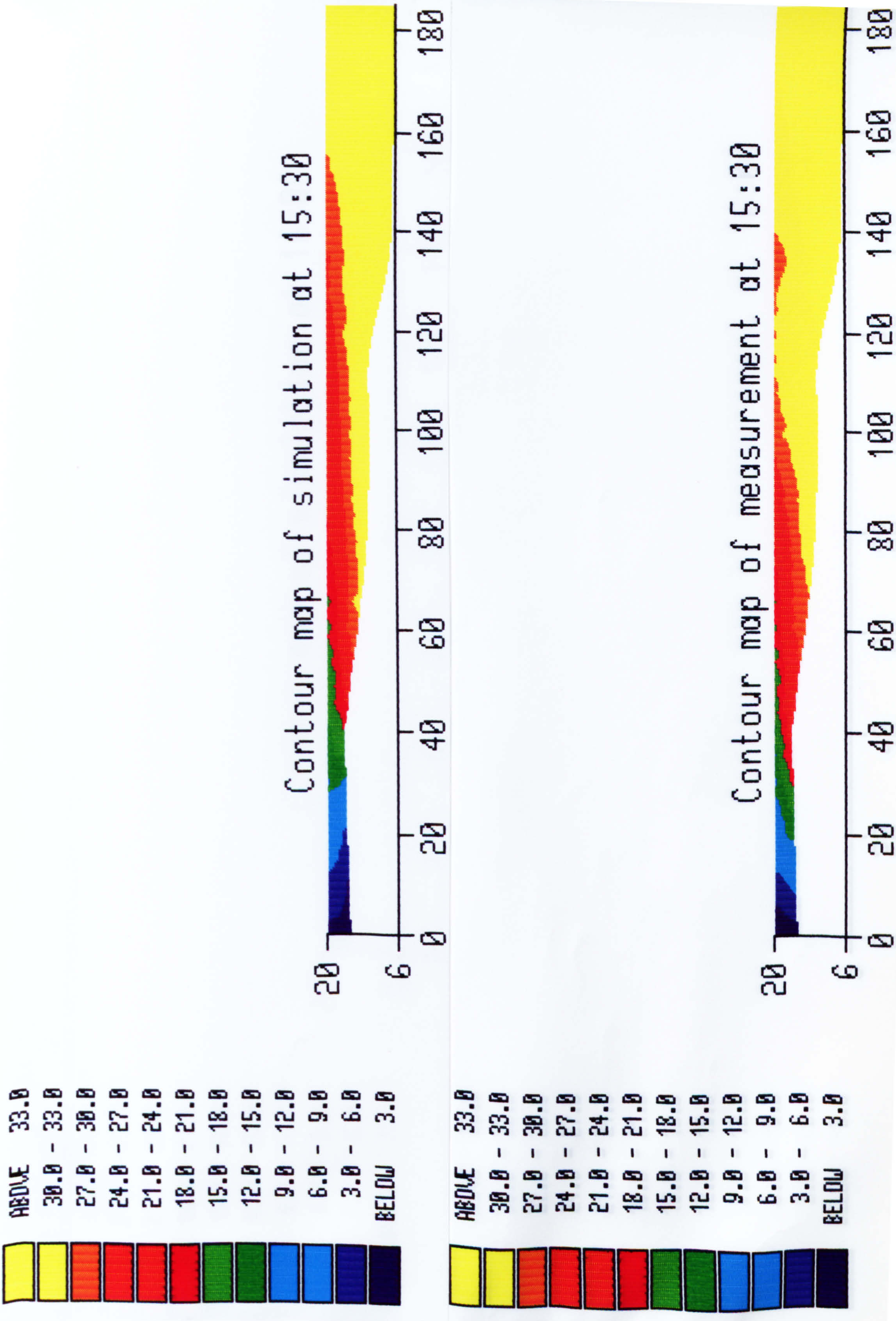

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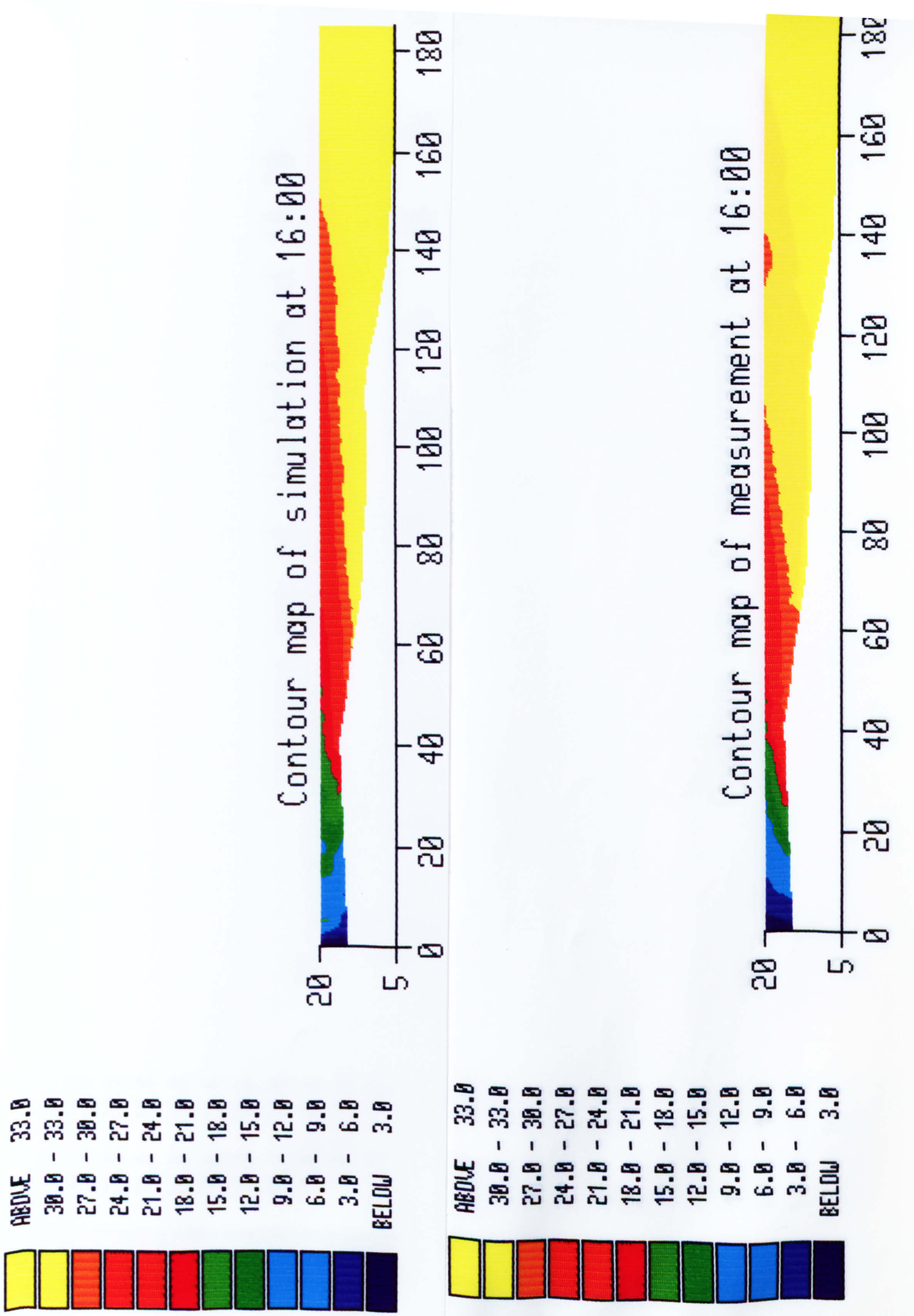

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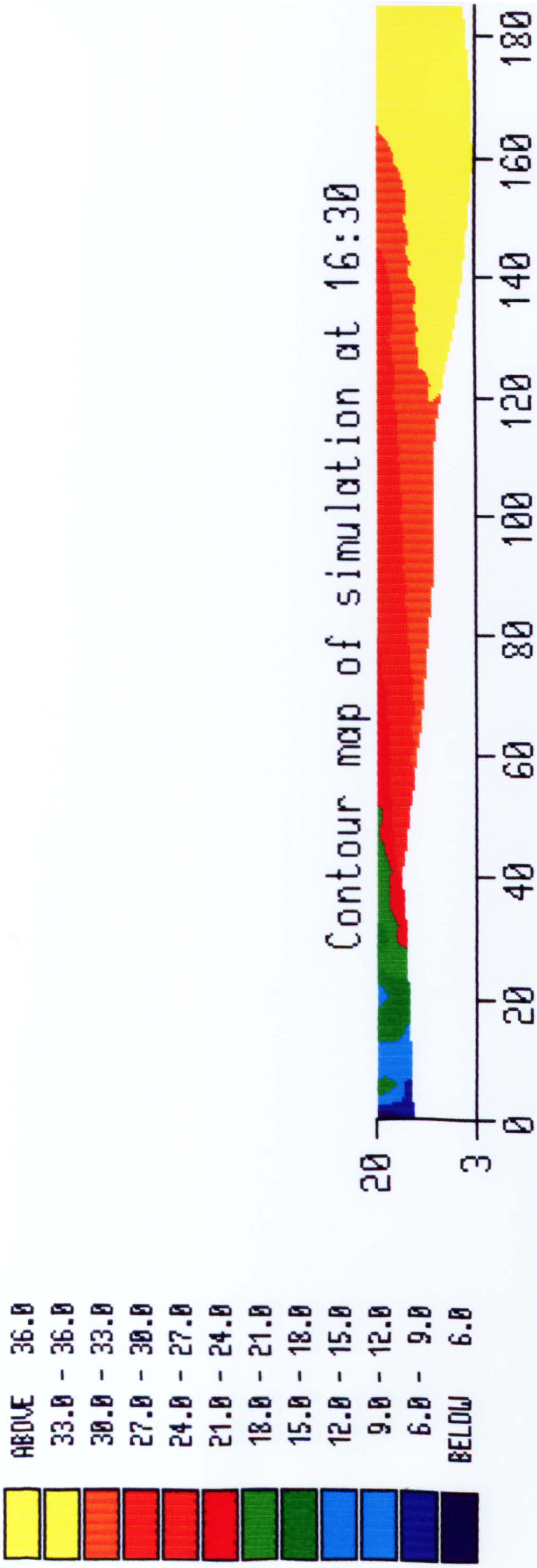


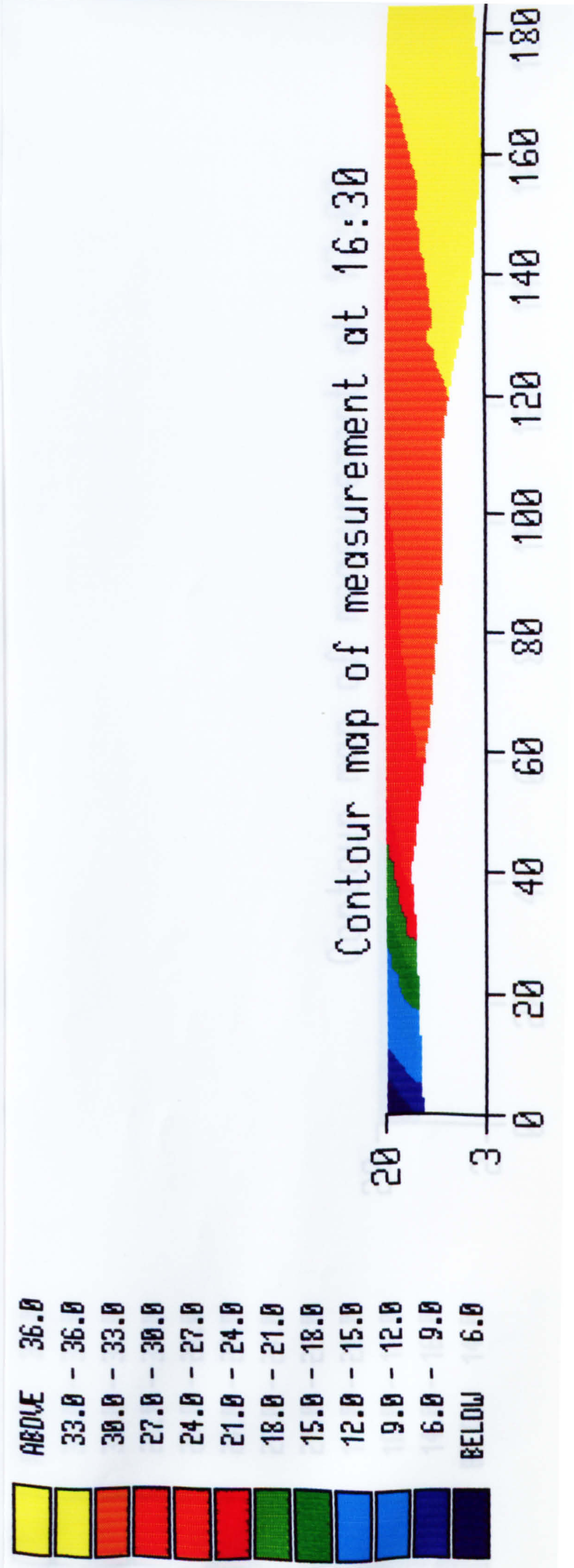
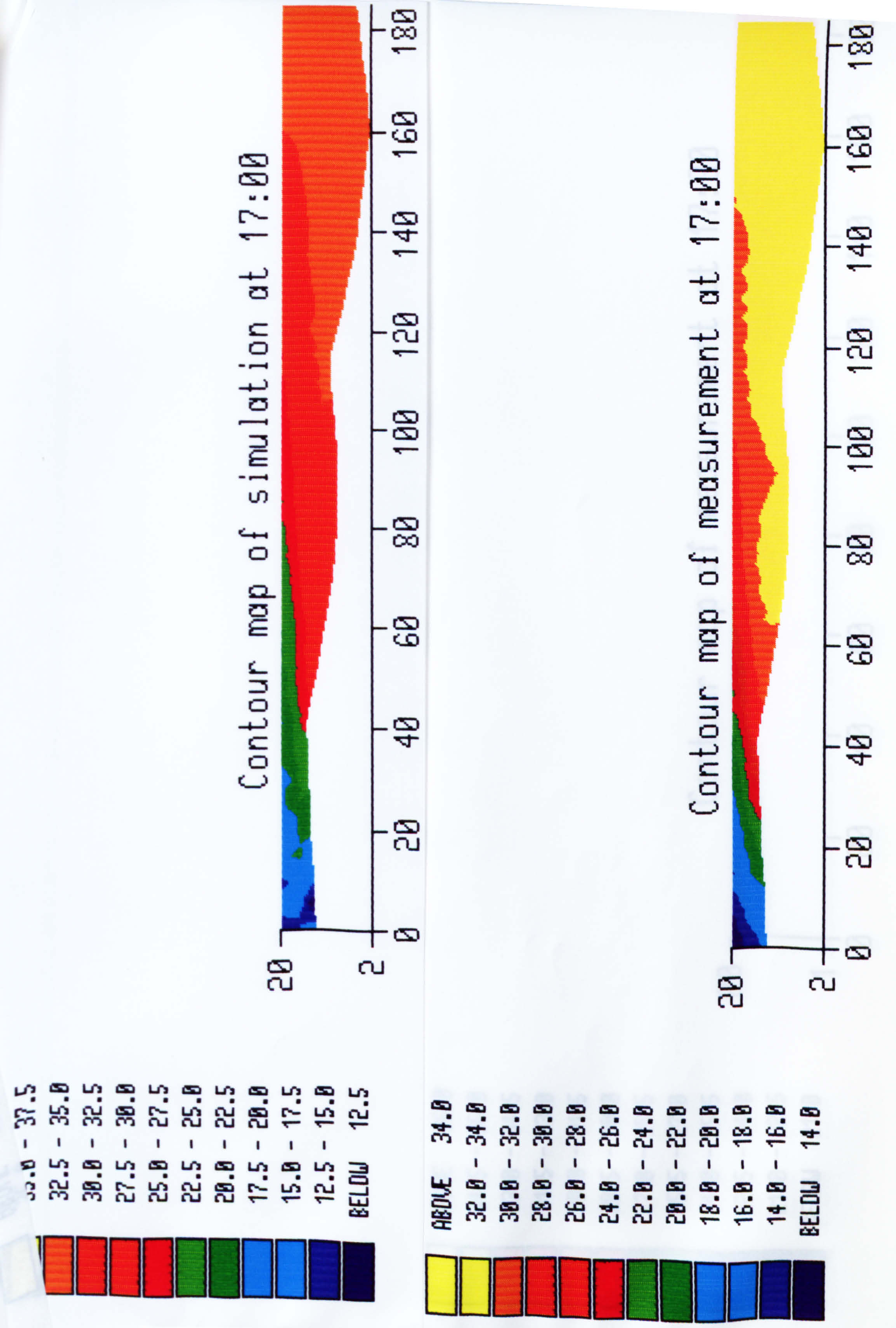


Fig. 7.59 Comparison between measurements and simulations



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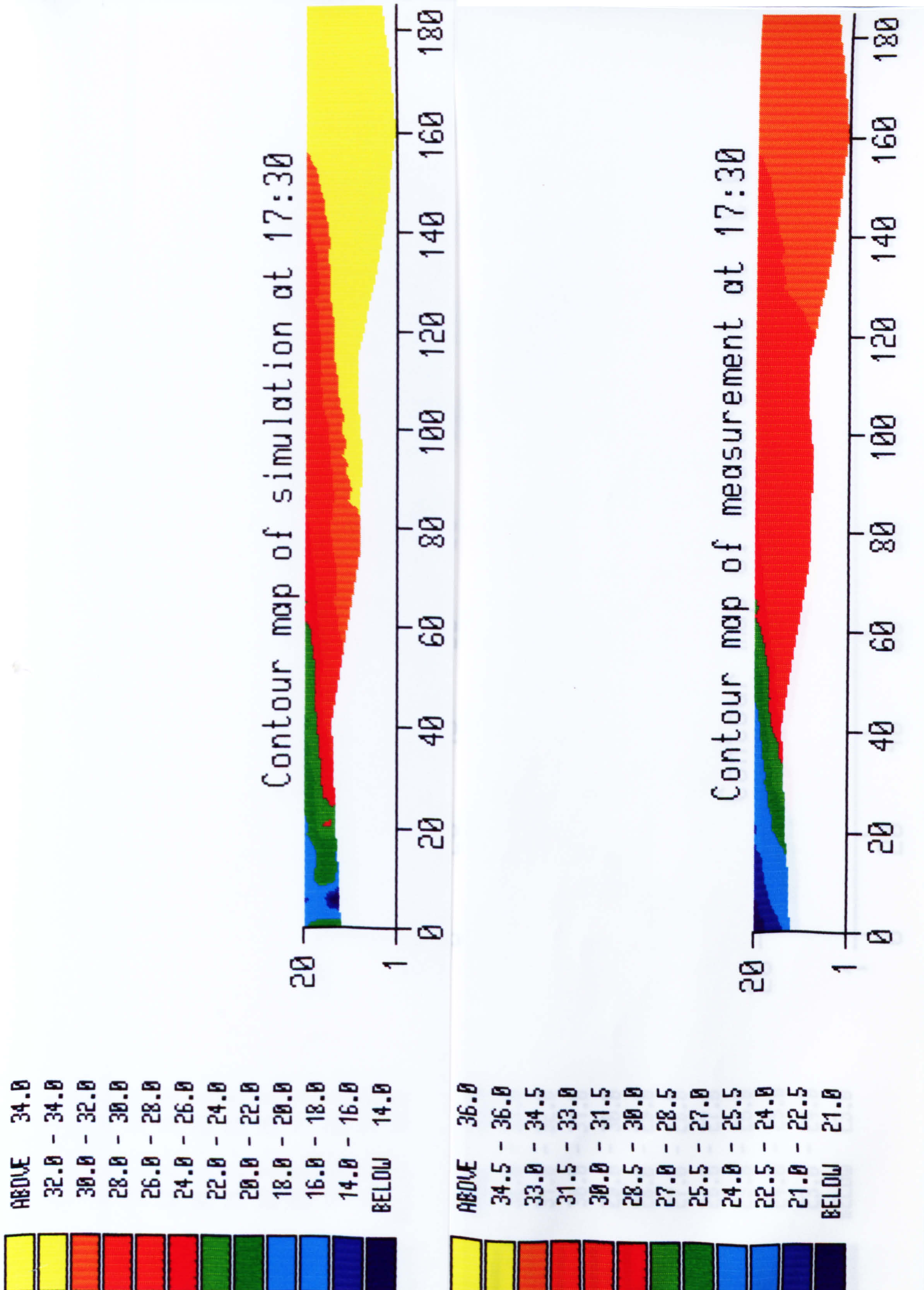

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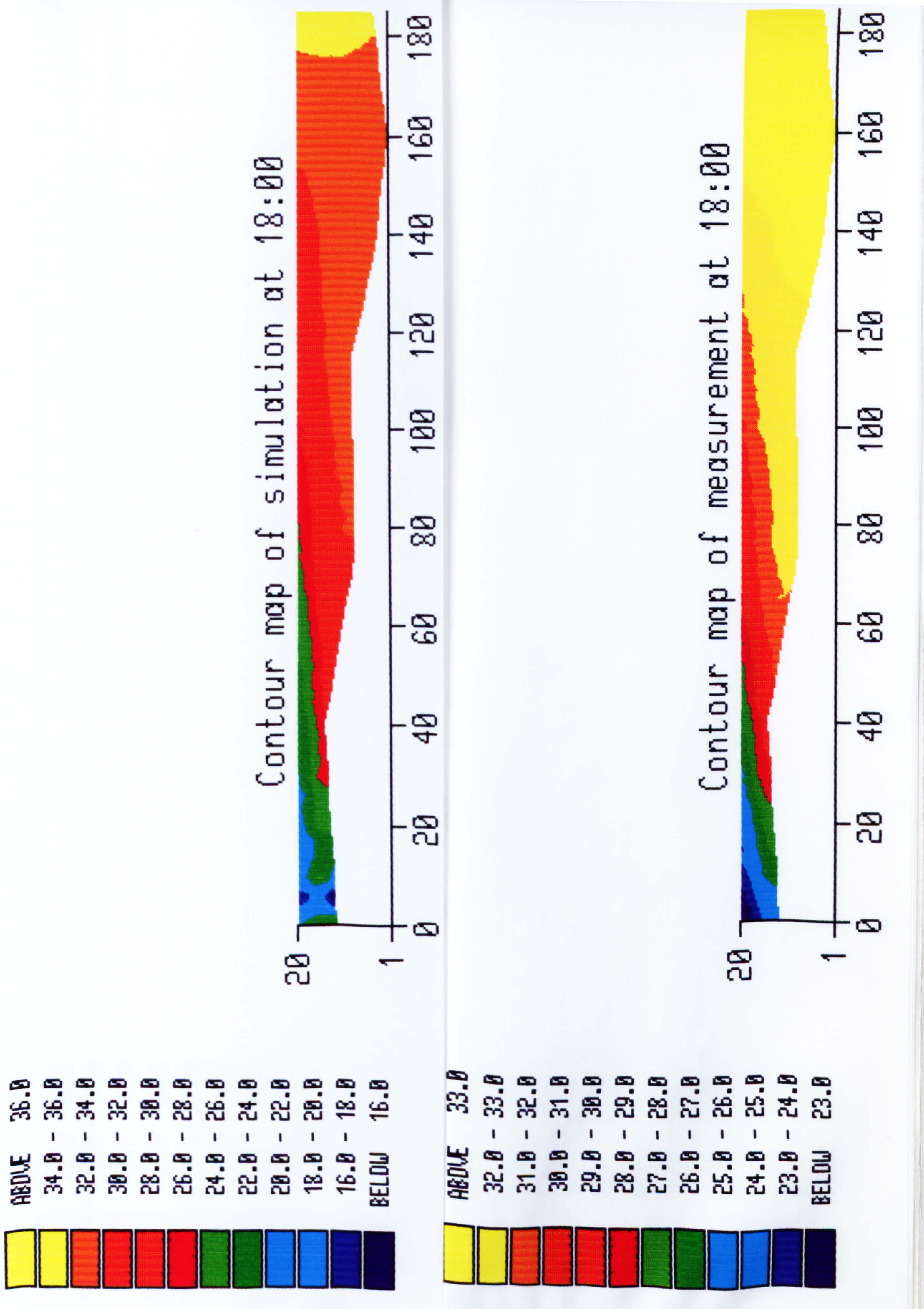

Fig. 7.62 Comparison between measurements and simulations

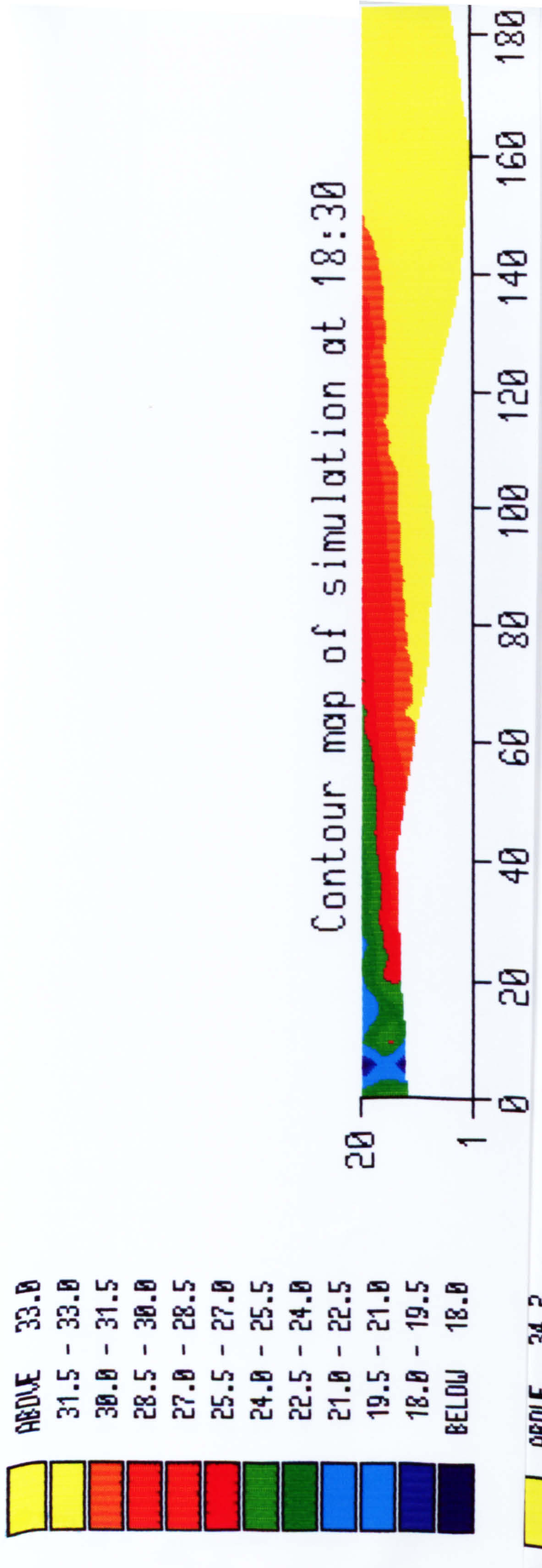

Fig. 7.63 Comparison between measurements and simulations

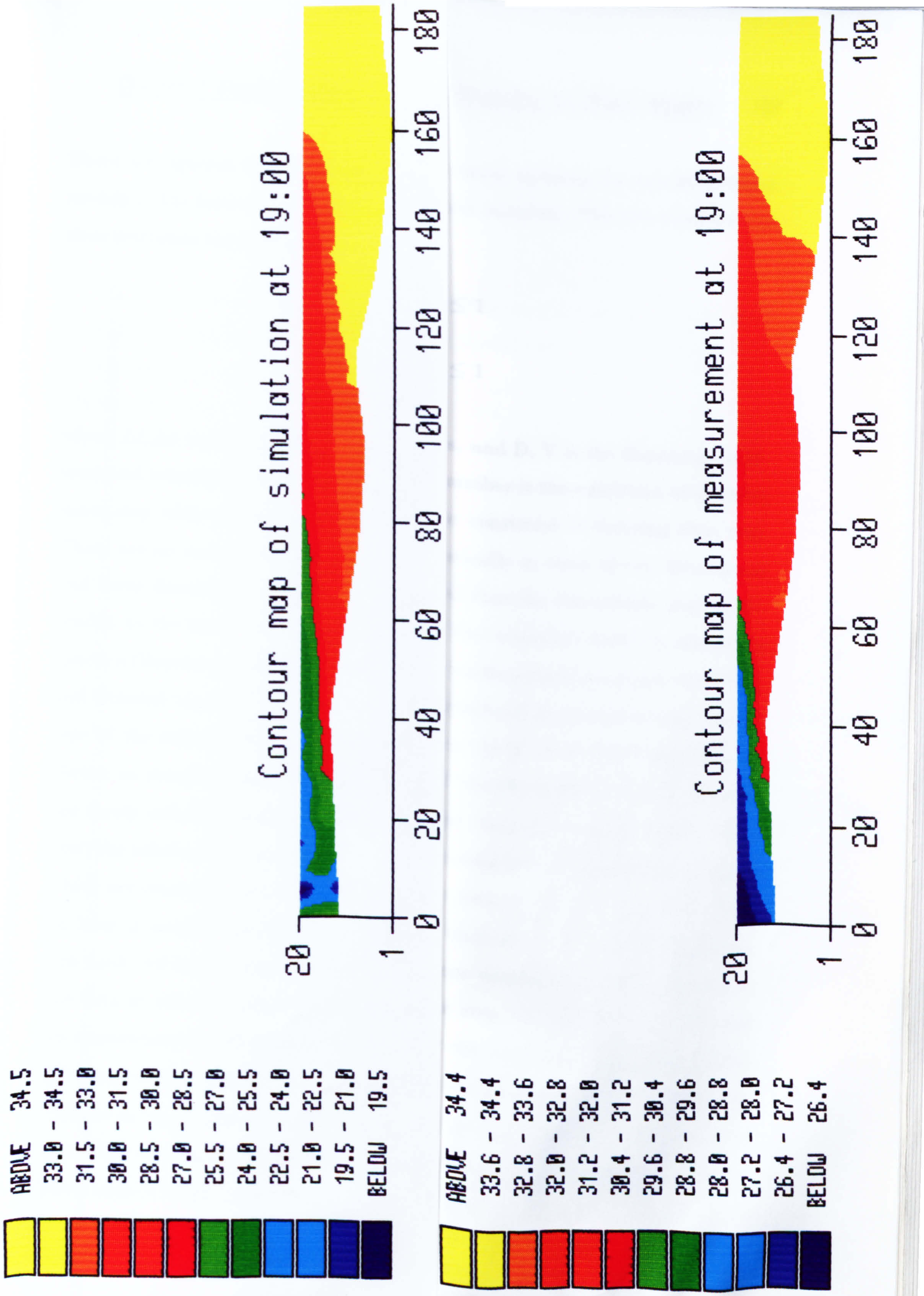

Fig. 7.64 Comparison between measurements and simulations

There are rigorous criteria to guarantee solution accuracy for one dimensional models in the form of the Peclet and Courant numbers. The two numbers and their restraints are expressed as

$$Pe = \frac{V\Delta l}{D} \leq 1$$

$$Cr = \frac{V\Delta t}{\Delta l} \leq 1$$

where $\Delta l, \Delta t$ represent space and time steps, and D, V is the dispersion coefficient and velocity respectively. The Peclet number is the constraint of choosing space step while the Courant number is the constraint of choosing time step. There are no such criteria derived mathematically in cases of two dimensional and three dimensional models. It is assumed that the two criteria may be extended to the latter cases analogously and the restraints could be relaxed in practice (Huyakorn and Pinder, 1983). Even under relaxed restraints, the Peclet and Courant numbers should not still be considered as stringent rules. In the case of the salinity simulation, the time step Δt is 0.5 hr and space step Δl chosen as $\max(\Delta x, \Delta y)$ 500m, the values of the Peclet and Courant numbers are rarely satisfied and are even much larger than the relaxed values. However, the solution results showed no obvious indications of numerical oscillations which are caused by the violation of the two criteria. As the time step of half an hour is usually regarded as too large, a time step of a quarter of an hour was used. All input data at the new time steps were linearly interpolated from the data at old time steps. With a finer time step, the solution results showed no improvements. All solutions showed that the numerical scheme was stable. By being stable, it means that the growth of the cumulative round-off errors induced during algebraic manipulations is controlled. This is because the time derivative term in the advection-dispersion equation is replaced by a fully implicit scheme which ensures the solution unconditionally stable. Therefore, the entire numerical scheme does not produce considerable solution errors. Those discrepancies between the simulation results and field measurements must be caused by another type of factor.

To obtain useful results, the model should be supplied all the data to define its structure. The input data for an estuary model are:
(1) Geographical data
(2) Velocity data
(3) Boundary condition data
(4) Mixing coefficient data
(5) Initial condition data

If any one of the data is inaccurately specified, the model results can be affected. The proceeding sections have described the preparations for each of them. Among these data, the boundary condition data are most susceptible and should be checked first. When the boundary condition data were prepared, the boundary conditions seaward and landward were regarded as the Dirichlet type, i.e., concentration prescribed. This boundary condition can be adopted if the boundary is located at the position where concentration gradients tend to zero or insignificant. Otherwise, the Neumann type of boundary conditions, i.e. flux of concentration prescribed, ought to be adopted. The validity of the Dirichlet type of boundary conditions will be checked next. At the seaward boundary, salinity concentrations approximate sea water concentrations so the salinity concentration gradient become almost zero there all the time. Hence, the boundary condition seaward is correctly satisfied. This may be the main reason why the simulation results are always accurate along the seaward part covering nearly half the whole simulation region. At the landward boundary, the salinity concentration changes from 27 ppm to 0 ppm and vice versa so that the salinity concentration gradient varies in the following manner:

(1) at first three hours between 6:30-9:30, the concentration gradient is insignificant(see Fig. 7.3-7.8)

(2) at next two and half hrs between 9:30-12:00, the concentration gradient increases to a significant level(see Fig. 7.9-7.13)

(3) at next two hrs between 12:00-14:00, the concentration gradient decreases to a insignificant level(see Fig. 7.14-17)

(4) at last two time intervals of 14:00-17:00 and 17:00-19:00, the concentration gradient behaves the same as the two proceeding intervals(see Fig. 7.18-7.27)

The above changes in salinity gradient at the upstream boundary meant that the Dirichlet condition was not always met throughout the tidal cycle. It is likely that this inadequacy in the boundary description was a contributing factor to the discrepancies between simulated and measured salinity profiles. Another source of error may be due to the poor representation of dispersion coefficient values. The model was tested with a range of values(factor of 10) to try and improve the fit of the predicted salinity. The model was found to be insensitive to changes in dispersion coefficient values within the range specified. It was found that salinity distribution was sensitive to changes in the velocity field. As was shown in Farraday's work, this study also noticed the sensitive role of the vertical diffusion coefficient in determining the extent of stratification in partially mixed estuaries. Within the range of 0.1-1.0 m^2/hr, the salinity distribution varied from highly stratified to well mixed. Compared with the salinity measurements, the appropriate stratification was achieved by a value of the vertical diffusion coefficient 0.5 m^2/hr.

An improved fit in the salinity data may be achieved by moving the upstream boundary to the tidal limit where the salinity is zero and the Dirichlet boundary condition is met. However, more survey data upstream of the existing boundary would be required to define the salinity and velocity fields. The alternative approach of specifying the salinity flux at the boundary, to satisfy the Neumann condition, was attempted using an approximation to the spatial salinity gradient at the boundary. No improvement in the salinity fit was achieved with this approach.

Chapter 8 Conclusions and Recommendations

Two important fields of estuarine pollution research: surveying and modelling have been studied in this thesis. The results of the study can be of considerable significance to the improvement of a surveying plan and modelling accuracy and reliability. The conclusions drawn from the study are summarized together with the recommendations for further research as following.

Methodology

The Kriging technique and the finite element method have been used for data estimations and solutions of the advection-dispersion equations respectively. This is the first time to apply the Kriging technique to estuarine surveying and modelling. As the variables of estuarine data belong to the class of non-stationary regionalized variables, generalized Kriging has been found to be the most suitable method to be employed. With the modified execution mode of the AKRIP package, generalized Kriging can be used with great ease. Especially, it is highly convenient to deal with large sets of data. In this study, 26 sets of salinity and velocity data must be estimated just for one tidal cycle. It has been shown that reliable estimations can be provided by the Kriging technique. The finite element method is a widely used numerical method for various problems involving computational solutions. In estuarine modelling, this study like other similar studies, has demonstrated the merits of applying this powerful numerical method.

Surveying

Analysis of the 1975 survey data by Kriging suggests that sampling effort for salinity should concentrate on the reaches with the steepest salinity gradient. The reestimation procedure showed that salinity and tempereature profiles could be characterised with fewer stations overall than used in 1975 survey. Intermediate stations could be reestimated within 5% of the measured values. Reestimation of velocity and dissolved oxygen could not reproduce at any of the eight stations within 5% of the original measured values suggesting that more stations were required to monitor these parameters.

Modelling

The most important part of estuarine modelling is the determination of velocity field, but it is also the most difficult part due to the complicated mechanisms involved. A new approach was developed to tackle this problem. It is the first time that field velocity data has been used in a direct way as input to a water quality model. This was made possible by means of the Kriging technique. This new approach together with the model was verified by the simulation of salinity intrusions. The simulation results showed an accurate reproduction of vertical and longitudinal salinity structure. It was found that the simulation was insensitive to the variation of the longitudinal dispersion coefficient but was sensitive to the variation of the advection term. This indicated that the longitudinal dispersion played a less important role in mass transport than the advection in the two dimensional laterally averaged model, which meant an accurate representation of the advection term is required, i.e., flow field specification is vital for accurate simulation results.

From the simulation, it was proved that this new approach was capable of providing accurate velocity fields in which they were measured on basis of a proper amount of data. It should be pointed out that any applications should be limited to the flow conditions which are similiar to the measured flow fields. By comparision, a hydrodynamical model may provide velocity fields in which tentative predictions could be made, in particular, following the change of physical geometry in an estuary. However, if the field velocity data represent typical flow patterns in the estuary, predictions can be made of overall water quality by applying the Kriging-finite element model of water quality. Untill hydrodynamic models become rigorous and predictive, this study offers a good alternative approach to the problem of flow field definition.

Recommendations

From this research project, the following recommendations are made

(1) The concentration of dissolved oxygen varies erratically in the estuary so that more sampling stations are required in order to know its full spatial distribution. The study conducted could only detect the insufficiency of sampling stations. It is necessary to know how many stations should be used and where they should be positioned. One possible way to do this is to analyse the simulation results of dissolved oxygen from a water quality model to find out the optimal sampling stations.

(2) The allocation of sampling stations along the estuary has been investigated. However, sometimes the surveying is also carried out for a certain purpose, e.g., to know discharge or fluxes of solute in a cross section. It is also necessary to know how many stations should be used and where they should be placed in the cross section. In this case, the Kriging technique will be as useful as it was shown in the previous study.

(3) The Kriging technique is able to provide satisfactory estimations, but it can not quantify its estimation errors. Therefore, if the estimation errors can be quantified and then are added in the estimations, more accurate estimations can be obtained. Conditional simulation is the technique with such a capacity. Thus, it is worthwhile applying it to estuarine surveying and modelling.

(4) The Kriging technique is computationally consumptive because of solving large sets of algebraic equations with frequent iterations. Particularly, if there are many sets of data and each set of data consists of a larger number of data points, then the computing will be turned into a formidable problem. Water

quality models will run into the same trouble if the models are two or three dimensional and are used for long-term simulations. This is a challenging problem. The only possible way is to reduce their CPU time. Normally, the most efficient solution method ought to be used if available so that the CPU time may be reduced. Recent developments in computing sciences have brought the encouraging news of parallel computing which is a breakthrough to the normal sequential computing. In parallel computing, the new powerful parallel computers execute many instructions of specially prepared programs concurrently so that the computing performance can be tremendously increased up to a factor as high as dozens depending on types of programmes. The specially prepared program may be a normal program which has been vectorized by the system (vector processor) or a program which has been written or compiled in a purpose-built concurrent programming language. Therefore, the programmers are responsible for producing programs which make the best use of the parallelism which exists. Many types of computers possess the parallel facility ranging from large scale supercomputers to small scale transputers. Therefore, if such computing facilities become available, it is worthwhile exploiting the potentiality of improving the programs performance.

(5) Hydrodynamic models in partially stratified estuaries can be established and be solved theoretically without any difficulties, but their applicability has been prohibited due to lack of representative model parameters. To obtain representative or predictive parameters, the mechanisms represented by them should be investigated thoroughly first. Hopefully, some research has been done in this respect though fewer quantitative results have been produced. Therefore, more efforts should be devoted to this research before turning out valid hydrodynamic models.

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User Instructions for the Program ESTUARY

The program ESTUARY is designed for the solution of the laterally integrated two dimensional advection-dispersion equation in partially mixed estuaries. The feature of the model is its direct input of velocity data which are prepared by the Kriging technique. Though the program is used for the simulation of salinity intrusion in the River Tees, it can be adapted for the simulation of other solutes like DO, BOD etc..

The flow chart of the program ESTUARY is shown in Fig. 6.2. The model parameters are classified as (1) input data parameters (2) program related parameters. They are listed as follows.

Imput Data Parametrs

NX	:	number of nodes along X direction
NY	:	number of nodes along Y direction
NC	:	number of nodes of prescribed salinity concentration
LC(I), I=1,NC	:	node number of prescribed salinity concentration
C(LC(I)), I=1,NC	:	prescribed salinity concentration(ppm)
C(I), I=1,228	:	initial salinity concentration(ppm)
DX	:	longitudinal dispersion coefficient(m^2/hr)
DY	:	vertical diffusion coefficient(m^2/hr)
NTS	:	number of time step
TSS	:	time step interval(hr)
WC	:	weighting coefficient(0.0-1.0) of stiffness matrix
U(I), I=1,228	:	longitudinal velocity component at node I (m/hr)
X(I), Y(I), I=1,228	:	X, Y coordinates at node I.

Program Related Parameters

NN	:	number of node
NE	:	number of elements
NB	:	half-band width of the global matrix
NKI(K,I)	:	node number of element K at node I
AM(I,J)	:	a component of global coefficients matrix at Ith line, Jth column

The data input channel is set up as channel 5, and the output channel is set up as channel 6. The solution results at each node are stored in the output file of channel 6 at each time step.

The Modified Execution Mode of the AKRIP

The original program of the AKRIP is an interactive program that leaves to the user much freedom in performing structure identification(see 4.2). The three steps of structure identification have been programmed as option A, option B and option C. Option A is to identify the order of the intrinsic random function. Option B is to determine the coefficients of the generalized covariance models that should be considered for every order of the intrinsic random function. Option C is to assess how well a given order of intrinsic random function and a given generalized covariance describe the data.

In an interactive mode, the option next can only be performed after the user chooses and inputs the result from the previous option. This does not cause any problem when a small amount of data needs to be processed. However, it may be a tedious process if a large amount of data must be processed. In this case, the program should be designed to run in a batch mode. Thus, the result from the previous option must be assigned to the next option as its input. A particular attention should be paid to the choice of the number of iterations to reach stable values of any generalized covariance model. In this study, ten iterations were set in the program.

Lists of Velocity Estimations and Variances by Kriging

and

Simulated and Kriged Salinity Values at the Following

Time: 8:00, 11:00,13:00, 15:00,18:00

STEP= 3 TIME= 8:00 hr

X (km)	Y (m)	U (m/s)	Variance (m/s)	Simulated (ppm)	Kriged (ppm)	Difference (ppm)
0.0	0.0	0.54534	0.00263	26.30	26.30	0.0
0.0	1.52	0.55478	0.00260	26.59	26.59	0.0
0.0	3.04	0.54294	0.00040	26.60	26.60	0.0
0.0	4.56	0.59332	0.00257	26.51	26.51	0.0
0.0	6.08	0.46303	0.00077	26.50	26.50	0.0
0.0	7.60	0.0	0.0	26.80	26.80	0.0
0.50	0.0	0.56249	0.00512	26.34	26.40	-0.06
0.50	1.47	0.56355	0.00437	26.63	26.80	-0.17
0.50	2.95	0.55827	0.00414	26.86	26.91	-0.05
0.50	4.42	0.58449	0.00436	26.92	26.97	-0.05
0.50	5.90	0.44731	0.00418	27.17	27.04	0.14
0.50	7.37	0.07722	0.00416	27.80	27.23	0.57
1.00	0.0	0.58095	0.00801	26.44	26.42	0.02
1.00	1.43	0.57353	0.00696	26.74	26.93	-0.19
1.00	2.86	0.56960	0.00695	27.15	27.21	-0.06
1.00	4.29	0.56355	0.00697	27.40	27.45	-0.05
1.00	5.72	0.42338	0.00705	27.87	27.62	0.25
1.00	7.15	0.13256	0.00730	28.43	27.79	0.65
1.50	0.0	0.59516	0.00983	26.58	26.41	0.18
1.50	1.38	0.58525	0.00868	26.90	27.01	-0.11
1.50	2.77	0.57871	0.00868	27.41	27.50	-0.09
1.50	4.15	0.54839	0.00869	27.82	27.92	-0.10
1.50	5.54	0.40231	0.00882	28.40	28.21	0.19
1.50	6.92	0.16117	0.00943	28.88	28.38	0.50
2.00	0.0	0.60583	0.01044	26.77	26.38	0.39
2.00	1.34	0.59695	0.00923	27.09	27.07	0.03
2.00	2.68	0.58709	0.00922	27.67	27.75	-0.07
2.00	4.02	0.54380	0.00922	28.21	28.36	-0.15
2.00	5.36	0.38759	0.00937	28.87	28.81	0.06
2.00	6.70	0.16812	0.01035	29.31	28.99	0.32
2.50	0.0	0.61290	0.00981	26.98	26.34	0.63
2.50	1.30	0.60762	0.00858	27.31	27.11	0.21
2.50	2.59	0.59493	0.00856	27.95	27.98	-0.03
2.50	3.89	0.55002	0.00857	28.57	28.75	-0.18
2.50	5.18	0.38559	0.00866	29.29	29.40	-0.10
2.50	6.48	0.15843	0.00994	29.74	29.61	0.13
3.00	0.0	0.61564	0.00798	27.20	26.29	0.91
3.00	1.25	0.61719	0.00680	27.54	27.14	0.41
3.00	2.50	0.60104	0.00682	28.22	28.20	0.02
3.00	3.75	0.56312	0.00681	28.90	29.08	-0.18
3.00	5.00	0.40880	0.00681	29.66	29.98	-0.32
3.00	6.25	0.13348	0.00811	30.13	30.21	-0.08
3.50	0.0	0.61255	0.00509	27.44	26.25	1.19
3.50	1.20	0.62668	0.00413	27.79	27.16	0.63
3.50	2.41	0.60341	0.00427	28.50	28.47	0.03
3.50	3.61	0.57358	0.00426	29.22	29.33	-0.11
3.50	4.82	0.47537	0.00411	29.98	30.54	-0.56
3.50	6.02	0.08806	0.00483	30.48	30.80	-0.33
4.00	0.0	0.60535	0.00252	27.69	26.33	1.37
4.00	1.16	0.63511	0.00140	28.03	27.20	0.83
4.00	2.32	0.60050	0.00227	28.76	28.81	-0.05
4.00	3.48	0.57121	0.00260	29.51	29.54	-0.03
4.00	4.64	0.53629	0.00240	30.24	30.94	-0.70
4.00	5.80	0.0	0.0	30.90	31.33	-0.43
4.50	0.0	0.60827	0.00491	27.93	26.76	1.17
4.50	1.32	0.61702	0.00411	28.40	27.91	0.48
4.50	2.64	0.57787	0.00414	29.32	29.32	-0.00
4.50	3.97	0.53530	0.00395	30.20	30.51	-0.31
4.50	5.29	0.31471	0.00397	31.05	31.64	-0.60
4.50	6.61	0.07194	0.00730	31.70	31.67	0.03
5.00	0.0	0.60738	0.00732	28.19	27.31	0.88

5.00	1.48	0.59688	0.00629	28.79	28.58	0.21
5.00	2.97	0.54523	0.00628	29.89	30.01	-0.12
5.00	4.45	0.45727	0.00628	30.88	31.33	-0.45
5.00	5.94	0.19030	0.00669	31.73	31.97	-0.23
5.00	7.42	0.13468	0.01027	32.12	31.98	0.14
5.50	0.0	0.60114	0.00836	28.46	27.84	0.62
5.50	1.65	0.57512	0.00725	29.20	29.21	-0.01
5.50	3.30	0.50076	0.00725	30.46	30.72	-0.26
5.50	4.94	0.37003	0.00725	31.49	31.87	-0.38
5.50	6.59	0.20640	0.00822	32.13	32.25	-0.12
5.50	8.24	0.19320	0.01027	32.33	32.27	0.06
6.00	0.0	0.59075	0.00790	28.74	28.35	0.39
6.00	1.81	0.55070	0.00680	29.61	29.80	-0.19
6.00	3.62	0.44885	0.00681	30.99	31.33	-0.34
6.00	5.43	0.32520	0.00685	31.95	32.24	-0.29
6.00	7.24	0.25796	0.00760	32.35	32.50	-0.15
6.00	9.05	0.23883	0.00843	32.42	32.51	-0.09
6.50	0.0	0.57578	0.00601	29.02	28.82	0.21
6.50	1.97	0.52233	0.00500	30.02	30.35	-0.33
6.50	3.94	0.39871	0.00500	31.46	31.78	-0.32
6.50	5.92	0.32059	0.00505	32.25	32.48	-0.23
6.50	7.89	0.31560	0.00533	32.45	32.70	-0.25
6.50	9.86	0.25513	0.00556	32.43	32.68	-0.25
7.00	0.0	0.55417	0.00310	29.31	29.24	0.07
7.00	2.13	0.48810	0.00209	30.42	30.83	-0.42
7.00	4.27	0.36289	0.00254	31.83	32.05	-0.22
7.00	6.40	0.34375	0.00286	32.43	32.61	-0.17
7.00	8.54	0.35964	0.00294	32.49	32.82	-0.33
7.00	10.67	0.11369	0.00275	32.39	32.60	-0.21
7.50	0.0	0.53014	0.00349	29.60	29.46	0.14
7.50	2.26	0.44640	0.00289	30.75	31.10	-0.36
7.50	4.52	0.35455	0.00317	32.06	32.13	-0.07
7.50	6.78	0.37717	0.00281	32.52	32.60	-0.07
7.50	9.04	0.37950	0.00253	32.49	32.79	-0.30
7.50	11.30	0.01565	0.00363	32.34	32.40	-0.06
8.00	0.0	0.50306	0.00546	29.87	29.51	0.36
8.00	2.36	0.40553	0.00470	31.01	31.18	-0.17
8.00	4.72	0.34908	0.00469	32.20	32.04	0.16
8.00	7.08	0.38639	0.00467	32.56	32.46	0.11
8.00	9.44	0.35537	0.00473	32.48	32.59	-0.11
8.00	11.80	0.02414	0.00659	32.32	32.30	0.01
8.50	0.0	0.47237	0.00545	30.13	29.54	0.59
8.50	2.46	0.36916	0.00470	31.22	31.19	0.03
8.50	4.92	0.34433	0.00466	32.29	31.88	0.41
8.50	7.38	0.38468	0.00470	32.57	32.27	0.30
8.50	9.84	0.29283	0.00468	32.46	32.34	0.12
8.50	12.30	0.01911	0.00659	32.32	32.31	0.01
9.00	0.0	0.44231	0.00348	30.36	29.54	0.82
9.00	2.56	0.34087	0.00315	31.40	31.20	0.19
9.00	5.12	0.34126	0.00261	32.34	31.73	0.60
9.00	7.68	0.37953	0.00300	32.57	32.11	0.45
9.00	10.24	0.23124	0.00285	32.44	32.16	0.28
9.00	12.80	0.00682	0.00363	32.35	32.40	-0.05
9.50	0.0	0.42999	0.00297	30.57	29.74	0.82
9.50	2.58	0.32930	0.00281	31.51	31.27	0.24
9.50	5.16	0.34047	0.00212	32.35	31.73	0.62
9.50	7.74	0.36649	0.00245	32.56	32.09	0.47
9.50	10.32	0.21155	0.00263	32.47	32.17	0.29
9.50	12.90	0.01238	0.00257	32.41	32.52	-0.11
10.00	0.0	0.44084	0.00508	30.74	30.22	0.52
10.00	2.48	0.33442	0.00438	31.56	31.41	0.15
10.00	4.96	0.33893	0.00430	32.33	31.89	0.43
10.00	7.44	0.34710	0.00438	32.56	32.24	0.32
10.00	9.92	0.23158	0.00431	32.52	32.37	0.16
10.00	12.40	0.03684	0.00607	32.49	32.60	-0.11
10.50	0.0	0.45299	0.00531	30.90	30.71	0.19

10.50	2.38	0.34595	0.00457	31.62	31.59	0.03
10.50	4.76	0.33311	0.00455	32.33	32.13	0.21
10.50	7.14	0.33748	0.00454	32.58	32.44	0.14
10.50	9.52	0.25517	0.00458	32.59	32.64	-0.05
10.50	11.90	0.04319	0.00632	32.59	32.73	-0.14
11.00	0.0	0.46137	0.00346	31.04	31.18	-0.14
11.00	2.28	0.35814	0.00291	31.69	31.78	-0.08
11.00	4.56	0.31601	0.00313	32.37	32.39	-0.02
11.00	6.84	0.33143	0.00267	32.63	32.65	-0.01
11.00	9.12	0.26500	0.00260	32.67	32.93	-0.26
11.00	11.40	0.02512	0.00356	32.72	32.93	-0.21
11.50	0.0	0.45337	0.00303	31.17	31.52	-0.34
11.50	2.29	0.34081	0.00259	31.81	32.02	-0.21
11.50	4.59	0.29069	0.00284	32.48	32.63	-0.15
11.50	6.88	0.30151	0.00201	32.73	32.86	-0.13
11.50	9.18	0.24708	0.00222	32.77	33.16	-0.38
11.50	11.47	0.01724	0.00369	32.90	33.12	-0.21
12.00	0.0	0.42555	0.00550	31.30	31.66	-0.37
12.00	2.48	0.28368	0.00478	32.01	32.32	-0.32
12.00	4.96	0.25638	0.00472	32.68	32.85	-0.17
12.00	7.45	0.24860	0.00478	32.87	33.09	-0.22
12.00	9.93	0.19128	0.00468	32.93	33.28	-0.35
12.00	12.41	0.04400	0.00798	33.12	33.22	-0.10
12.50	0.0	0.39370	0.00647	31.43	31.79	-0.37
12.50	2.67	0.22890	0.00589	32.22	32.59	-0.37
12.50	5.34	0.20481	0.00588	32.89	33.05	-0.16
12.50	8.01	0.21824	0.00572	33.03	33.26	-0.24
12.50	10.68	0.13293	0.00592	33.12	33.38	-0.26
12.50	13.35	0.05274	0.00815	33.31	33.33	-0.03
13.00	0.0	0.36319	0.00553	31.55	31.91	-0.36
13.00	2.86	0.17973	0.00575	32.45	32.81	-0.36
13.00	5.71	0.14788	0.00506	33.09	33.24	-0.14
13.00	8.57	0.19918	0.00546	33.18	33.39	-0.21
13.00	11.43	0.11923	0.00559	33.30	33.46	-0.17
13.00	14.29	0.04428	0.00579	33.49	33.46	0.02
13.50	0.0	0.33819	0.00304	31.70	32.02	-0.33
13.50	3.04	0.14448	0.00514	32.68	32.99	-0.31
13.50	6.09	0.09447	0.00203	33.29	33.40	-0.11
13.50	9.13	0.18083	0.00506	33.34	33.51	-0.16
13.50	12.18	0.12567	0.00245	33.47	33.56	-0.09
13.50	15.22	0.01371	0.00339	33.65	33.63	0.02
14.00	0.0	0.32788	0.00357	31.86	32.13	-0.27
14.00	3.20	0.13278	0.00511	32.89	33.13	-0.23
14.00	6.41	0.09055	0.00395	33.45	33.51	-0.06
14.00	9.61	0.16151	0.00384	33.50	33.62	-0.12
14.00	12.82	0.10884	0.00516	33.64	33.69	-0.05
14.00	16.02	-0.00288	0.00444	33.79	33.80	-0.01
14.50	0.0	0.33057	0.00589	32.04	32.22	-0.18
14.50	3.35	0.14494	0.00588	33.08	33.24	-0.15
14.50	6.69	0.09828	0.00592	33.59	33.61	-0.02
14.50	10.04	0.13043	0.00530	33.65	33.76	-0.11
14.50	13.39	0.08797	0.00585	33.80	33.84	-0.04
14.50	16.73	-0.00372	0.00803	33.91	33.94	-0.03
15.00	0.0	0.33950	0.00648	32.26	32.31	-0.05
15.00	3.49	0.17096	0.00613	33.26	33.33	-0.07
15.00	6.98	0.09920	0.00635	33.73	33.72	0.01
15.00	10.46	0.10026	0.00610	33.80	33.91	-0.11
15.00	13.95	0.06085	0.00588	33.94	34.00	-0.05
15.00	17.44	0.00086	0.00797	34.02	34.06	-0.04
15.50	0.0	0.35237	0.00513	32.50	32.38	0.11
15.50	3.63	0.20281	0.00494	33.44	33.43	0.01
15.50	7.26	0.09128	0.00559	33.86	33.84	0.01
15.50	10.89	0.08161	0.00573	33.94	34.05	-0.11
15.50	14.52	0.03669	0.00521	34.08	34.15	-0.07
15.50	18.15	0.00765	0.00502	34.12	34.15	-0.03
16.00	0.0	0.36699	0.00263	32.75	32.48	0.27

16.00	3.77	0.23423	0.00226	33.60	33.52	0.08
16.00	7.54	0.07591	0.00368	33.99	33.98	0.01
16.00	11.31	0.07618	0.00463	34.06	34.17	-0.11
16.00	15.09	0.02448	0.00506	34.21	34.28	-0.07
16.00	18.86	0.00225	0.00155	34.19	34.16	0.03
16.50	0.0	0.37939	0.00413	33.02	32.75	0.26
16.50	3.70	0.24249	0.00397	33.75	33.66	0.09
16.50	7.39	0.07475	0.00490	34.09	34.05	0.04
16.50	11.09	0.05837	0.00541	34.17	34.26	-0.10
16.50	14.79	0.02362	0.00524	34.30	34.36	-0.06
16.50	18.48	0.01796	0.00391	34.27	34.30	-0.03
17.00	0.0	0.39031	0.00618	33.27	33.10	0.17
17.00	3.57	0.24180	0.00587	33.89	33.81	0.08
17.00	7.13	0.08092	0.00621	34.20	34.11	0.09
17.00	10.70	0.05297	0.00611	34.26	34.33	-0.07
17.00	14.27	0.03130	0.00563	34.38	34.42	-0.04
17.00	17.84	0.02312	0.00684	34.37	34.42	-0.04
17.50	0.0	0.40021	0.00638	33.57	33.44	0.13
17.50	3.44	0.24013	0.00614	34.05	33.97	0.08
17.50	6.88	0.09073	0.00631	34.30	34.18	0.12
17.50	10.31	0.07156	0.00593	34.35	34.38	-0.03
17.50	13.75	0.04558	0.00586	34.45	34.47	-0.02
17.50	17.19	0.01778	0.00816	34.47	34.49	-0.03
18.00	0.0	0.40829	0.00468	33.75	33.78	-0.03
18.00	3.31	0.23956	0.00532	34.19	34.13	0.05
18.00	6.62	0.10761	0.00518	34.39	34.26	0.13
18.00	9.93	0.10571	0.00403	34.43	34.42	0.00
18.00	13.24	0.04419	0.00544	34.52	34.52	-0.01
18.00	16.55	0.00924	0.00613	34.54	34.55	-0.01
18.50	0.0	0.41161	0.00262	34.07	34.07	0.0
18.50	3.18	0.24440	0.00500	34.29	34.29	0.0
18.50	6.36	0.13056	0.00306	34.36	34.36	0.0
18.50	9.54	0.11174	0.00367	34.48	34.48	0.0
18.50	12.72	0.01524	0.00476	34.58	34.58	0.0
18.50	15.90	0.0	0.0	34.59	34.59	0.0

STEP= 9 TIME=11:00 hr

X (km)	Y (m)	U (m/s)	Variance (m/s)	Simulated (ppm)	Kriged (ppm)	Difference (ppm)
0.0	0.0	1.22764	0.01180	3.48	3.48	0.0
0.0	0.56	1.15257	0.00846	3.34	3.34	0.0
0.0	1.12	1.13883	0.00491	3.19	3.19	0.0
0.0	1.68	1.18275	0.01012	3.09	3.09	0.0
0.0	2.24	0.84562	0.00781	3.22	3.22	0.0
0.0	2.80	0.0	0.0	3.68	3.68	0.0
0.50	0.0	1.24403	0.02311	4.07	5.91	-1.85
0.50	0.56	1.16505	0.01861	4.04	5.81	-1.77
0.50	1.13	1.12515	0.01861	3.96	5.71	-1.75
0.50	1.69	1.05894	0.01928	3.99	5.65	-1.67
0.50	2.25	0.72900	0.01857	4.70	5.78	-1.08
0.50	2.81	0.20822	0.01936	5.69	6.10	-0.42
1.00	0.0	1.24412	0.03632	5.01	8.39	-3.38
1.00	0.56	1.15026	0.03180	5.04	8.35	-3.31
1.00	1.13	1.05955	0.03121	5.11	8.31	-3.20
1.00	1.69	0.91289	0.03124	5.50	8.30	-2.80
1.00	2.26	0.63235	0.03127	6.83	8.40	-1.56
1.00	2.82	0.27659	0.03312	7.97	8.59	-0.62
1.50	0.0	1.22323	0.04463	6.02	10.86	-4.83
1.50	0.57	1.11341	0.04026	6.13	10.90	-4.77
1.50	1.13	0.99008	0.03911	6.41	10.90	-4.49
1.50	1.70	0.81725	0.03898	7.29	10.91	-3.61
1.50	2.27	0.57164	0.03938	9.01	10.96	-1.94
1.50	2.84	0.28950	0.04147	10.19	11.05	-0.87
2.00	0.0	1.18917	0.04736	7.13	13.29	-6.17
2.00	0.57	1.07043	0.04296	7.31	13.40	-6.09
2.00	1.14	0.93444	0.04158	7.87	13.44	-5.57
2.00	1.71	0.75665	0.04140	9.16	13.44	-4.28
2.00	2.28	0.52899	0.04197	11.15	13.43	-2.28
2.00	2.85	0.27959	0.04413	12.35	13.45	-1.10
2.50	0.0	1.14731	0.04440	8.32	15.67	-7.35
2.50	0.57	1.02908	0.03983	8.61	15.85	-7.24
2.50	1.14	0.89675	0.03852	9.44	15.90	-6.46
2.50	1.72	0.72335	0.03839	11.11	15.87	-4.76
2.50	2.29	0.49878	0.03893	13.26	15.80	-2.55
2.50	2.86	0.25572	0.04111	14.44	15.74	-1.30
3.00	0.0	1.09862	0.03601	9.62	17.97	-8.35
3.00	0.57	0.99015	0.03120	9.98	18.21	-8.23
3.00	1.15	0.87870	0.03040	11.03	18.25	-7.22
3.00	1.72	0.72056	0.03041	12.86	18.18	-5.32
3.00	2.30	0.48192	0.03068	15.15	18.04	-2.88
3.00	2.87	0.21534	0.03265	16.42	17.89	-1.47
3.50	0.0	1.04083	0.02290	10.99	20.14	-9.15
3.50	0.58	0.94894	0.01824	11.43	20.45	-9.01
3.50	1.15	0.87817	0.01822	12.62	20.44	-7.82
3.50	1.73	0.76078	0.01865	14.62	20.30	-5.69
3.50	2.31	0.48675	0.01855	16.97	20.10	-3.13
3.50	2.89	0.14219	0.01914	18.14	19.87	-1.72
4.00	0.0	0.98389	0.01129	12.44	22.05	-9.61
4.00	0.58	0.90815	0.00859	12.89	22.38	-9.49
4.00	1.16	0.87596	0.00625	14.08	22.33	-8.25
4.00	1.74	0.81891	0.00894	15.98	22.15	-6.17
4.00	2.32	0.51169	0.00958	18.37	21.90	-3.53
4.00	2.90	0.0	0.0	20.26	21.62	-1.36
4.50	0.0	0.97491	0.02198	13.82	23.32	-9.50
4.50	0.77	0.87787	0.01751	14.58	23.69	-9.11
4.50	1.54	0.78949	0.01862	16.60	23.61	-7.00
4.50	2.31	0.50378	0.01802	19.79	23.36	-3.57
4.50	3.08	0.12642	0.02000	23.23	23.07	0.16
4.50	3.85	0.01805	0.03607	25.60	22.87	2.72
5.00	0.0	0.96555	0.03279	15.12	24.32	-9.20

5.00	0.96	0.82984	0.02798	16.25	24.71	-8.45
5.00	1.92	0.64088	0.02794	19.28	24.64	-5.35
5.00	2.88	0.31159	0.02909	23.50	24.41	-0.91
5.00	3.84	0.12422	0.03819	27.04	24.25	2.79
5.00	4.81	0.04365	0.04973	28.90	24.17	4.74
5.50	0.0	0.94504	0.03742	16.35	25.18	-8.83
5.50	1.15	0.77518	0.03239	17.94	25.58	-7.64
5.50	2.30	0.54041	0.03244	21.87	25.55	-3.67
5.50	3.46	0.28500	0.03541	26.44	25.45	0.99
5.50	4.61	0.15703	0.04259	29.38	25.45	3.93
5.50	5.76	0.07456	0.04877	30.65	25.47	5.18
6.00	0.0	0.91558	0.03538	17.54	25.94	-8.40
6.00	1.34	0.73185	0.03034	19.56	26.33	-6.77
6.00	2.68	0.50375	0.03065	24.11	26.37	-2.27
6.00	4.03	0.30501	0.03311	28.49	26.50	1.99
6.00	5.37	0.19930	0.03661	30.73	26.62	4.11
6.00	6.71	0.09558	0.03974	31.55	26.76	4.79
6.50	0.0	0.87791	0.02687	18.68	26.61	-7.92
6.50	1.53	0.70692	0.02263	21.08	26.96	-5.88
6.50	3.07	0.50199	0.02251	26.01	27.13	-1.13
6.50	4.60	0.34077	0.02382	29.91	27.50	2.41
6.50	6.13	0.23718	0.02455	31.50	27.76	3.74
6.50	7.67	0.07943	0.03077	32.02	27.76	4.26
7.00	0.0	0.83373	0.01387	19.78	27.18	-7.40
7.00	1.72	0.69609	0.01141	22.44	27.48	-5.04
7.00	3.45	0.50812	0.01297	27.48	27.85	-0.37
7.00	5.17	0.38118	0.00996	30.84	28.35	2.48
7.00	6.89	0.25917	0.00913	31.93	29.12	2.82
7.00	8.62	0.02184	0.01624	32.27	28.15	4.12
7.50	0.0	0.81635	0.01559	20.86	27.56	-6.70
7.50	1.80	0.68358	0.01232	23.43	27.85	-4.41
7.50	3.61	0.52654	0.01387	28.18	28.34	-0.16
7.50	5.41	0.41581	0.01395	31.18	28.85	2.34
7.50	7.21	0.25957	0.01374	32.11	29.70	2.41
7.50	9.01	0.00886	0.01187	32.34	28.70	3.64
8.00	0.0	0.81706	0.02436	21.86	27.78	-5.92
8.00	1.81	0.66010	0.02084	24.23	28.09	-3.86
8.00	3.62	0.54293	0.02097	28.54	28.55	-0.02
8.00	5.42	0.44358	0.02103	31.30	29.09	2.21
8.00	7.23	0.26011	0.02256	32.18	29.94	2.24
8.00	9.04	0.01574	0.02268	32.37	29.34	3.03
8.50	0.0	0.81260	0.02435	22.77	27.94	-5.17
8.50	1.81	0.63485	0.02080	24.99	28.28	-3.29
8.50	3.62	0.54828	0.02092	28.91	28.69	0.22
8.50	5.44	0.46032	0.02098	31.45	29.19	2.26
8.50	7.25	0.24525	0.02267	32.25	30.16	2.08
8.50	9.06	0.01424	0.02268	32.38	29.86	2.52
9.00	0.0	0.80636	0.01555	23.60	28.07	-4.47
9.00	1.82	0.61412	0.01217	25.73	28.46	-2.73
9.00	3.63	0.55074	0.01369	29.29	28.83	0.46
9.00	5.45	0.46969	0.01406	31.59	29.26	2.32
9.00	7.27	0.21683	0.01481	32.30	30.43	1.87
9.00	9.09	0.00660	0.01187	32.39	30.29	2.10
9.50	0.0	0.79476	0.01327	24.38	28.36	-3.97
9.50	1.79	0.61223	0.01018	26.36	28.74	-2.38
9.50	3.58	0.55816	0.01251	29.56	29.10	0.46
9.50	5.38	0.47124	0.01224	31.66	29.54	2.12
9.50	7.17	0.20585	0.01035	32.32	30.73	1.59
9.50	8.96	0.01128	0.01003	32.40	30.69	1.71
10.00	0.0	0.77490	0.02269	25.12	28.85	-3.73
10.00	1.72	0.63138	0.01937	26.86	29.13	-2.27
10.00	3.44	0.57461	0.01951	29.66	29.50	0.16
10.00	5.17	0.47666	0.01925	31.61	30.04	1.56
10.00	6.89	0.23836	0.01943	32.31	31.06	1.24
10.00	8.61	0.02894	0.02448	32.42	31.07	1.35
10.50	0.0	0.75338	0.02368	25.81	29.33	-3.52

10.50	1.65	0.65275	0.02034	27.31	29.53	-2.22
10.50	3.30	0.59110	0.02031	29.76	29.92	-0.15
10.50	4.96	0.48608	0.02017	31.56	30.54	1.02
10.50	6.61	0.26270	0.02038	32.29	31.53	0.76
10.50	8.26	0.03272	0.02570	32.44	31.39	1.04
11.00	0.0	0.72702	0.01544	26.46	29.74	-3.28
11.00	1.58	0.66289	0.01388	27.73	29.87	-2.14
11.00	3.16	0.59102	0.01194	29.87	30.27	-0.40
11.00	4.75	0.49452	0.01276	31.52	30.88	0.64
11.00	6.33	0.27209	0.01337	32.27	31.99	0.28
11.00	7.91	0.02008	0.01404	32.47	31.70	0.77
11.50	0.0	0.70406	0.01352	27.05	29.97	-2.92
11.50	1.61	0.63966	0.01250	28.24	30.08	-1.84
11.50	3.22	0.54960	0.01050	30.25	30.52	-0.26
11.50	4.83	0.44093	0.00973	31.73	31.16	0.57
11.50	6.44	0.22507	0.01279	32.37	32.19	0.18
11.50	8.05	0.00085	0.01576	32.61	31.67	0.94
12.00	0.0	0.68860	0.02455	27.58	30.00	-2.42
12.00	1.78	0.56826	0.02096	28.89	30.16	-1.26
12.00	3.57	0.45701	0.02125	30.94	30.68	0.26
12.00	5.35	0.30087	0.02125	32.16	31.47	0.69
12.00	7.14	0.11159	0.02073	32.61	31.87	0.75
12.00	8.92	0.00770	0.03513	32.90	31.31	1.59
12.50	0.0	0.67088	0.02888	28.09	29.97	-1.88
12.50	1.96	0.47243	0.02542	29.55	30.19	-0.63
12.50	3.92	0.34009	0.02550	31.55	30.75	0.80
12.50	5.88	0.18573	0.02552	32.47	31.43	1.05
12.50	7.84	0.05795	0.02655	32.87	31.38	1.49
12.50	9.80	0.01705	0.03557	33.16	31.20	1.96
13.00	0.0	0.65405	0.02466	28.56	29.90	-1.34
13.00	2.13	0.36822	0.02183	30.19	30.23	-0.04
13.00	4.27	0.22704	0.02245	32.05	30.79	1.26
13.00	6.40	0.10900	0.02325	32.72	31.21	1.52
13.00	8.54	0.06235	0.02567	33.10	31.10	2.00
13.00	10.67	0.01834	0.02888	33.38	31.50	1.88
13.50	0.0	0.64292	0.01355	29.04	29.86	-0.82
13.50	2.31	0.27776	0.01383	30.80	30.39	0.42
13.50	4.62	0.15179	0.02005	32.43	30.92	1.51
13.50	6.93	0.08849	0.02282	32.94	31.17	1.77
13.50	9.24	0.07887	0.02228	33.29	31.15	2.14
13.50	11.55	0.00639	0.01518	33.57	32.25	1.33
14.00	0.0	0.63745	0.01591	29.47	30.23	-0.76
14.00	2.48	0.26420	0.01878	31.28	30.82	0.46
14.00	4.95	0.13011	0.02350	32.71	31.27	1.44
14.00	7.43	0.10436	0.02022	33.12	31.35	1.76
14.00	9.91	0.09082	0.01233	33.46	31.47	1.99
14.00	12.39	-0.01074	0.02145	33.74	32.97	0.76
14.50	0.0	0.63833	0.02628	29.91	30.90	-0.99
14.50	2.64	0.29107	0.02615	31.63	31.43	0.21
14.50	5.28	0.13940	0.02649	32.92	31.80	1.12
14.50	7.92	0.12386	0.02365	33.28	31.88	1.39
14.50	10.56	0.08273	0.02558	33.61	32.41	1.20
14.50	13.20	-0.02504	0.03766	33.88	33.53	0.35
15.00	0.0	0.64433	0.02891	30.25	31.58	-1.33
15.00	2.80	0.32178	0.02814	31.91	32.11	-0.20
15.00	5.60	0.16356	0.02693	33.10	32.48	0.62
15.00	8.41	0.13592	0.02699	33.43	32.60	0.83
15.00	11.21	0.06318	0.02796	33.76	33.22	0.54
15.00	14.01	-0.02979	0.03548	34.01	33.91	0.10
15.50	0.0	0.64893	0.02291	30.62	32.22	-1.59
15.50	2.96	0.34109	0.02566	32.16	32.79	-0.63
15.50	5.93	0.18676	0.02012	33.26	33.20	0.07
15.50	8.89	0.13632	0.02556	33.58	33.29	0.30
15.50	11.86	0.03556	0.02044	33.92	33.81	0.11
15.50	14.82	-0.02303	0.02776	34.12	34.16	-0.05
16.00	0.0	0.63444	0.01177	30.88	32.78	-1.90

16.00	3.13	0.33408	0.02241	32.37	33.39	-1.02
16.00	6.25	0.19491	0.01088	33.42	33.82	-0.40
16.00	9.38	0.12381	0.01959	33.75	33.87	-0.12
16.00	12.51	0.00856	0.01765	34.06	34.18	-0.12
16.00	15.64	-0.00502	0.00806	34.19	34.30	-0.11
16.50	0.0	0.52417	0.01845	31.25	33.15	-1.89
16.50	3.09	0.29938	0.02414	32.53	33.79	-1.26
16.50	6.19	0.18505	0.01616	33.51	34.16	-0.65
16.50	9.28	0.09914	0.02301	33.88	34.20	-0.32
16.50	12.37	-0.00333	0.01859	34.15	34.37	-0.21
16.50	15.47	0.01717	0.01880	34.23	34.36	-0.13
17.00	0.0	0.36624	0.02760	31.50	33.39	-1.88
17.00	3.01	0.22733	0.02784	32.65	34.02	-1.37
17.00	6.02	0.15685	0.02495	33.61	34.30	-0.70
17.00	9.03	0.06437	0.02777	34.02	34.37	-0.34
17.00	12.04	-0.02141	0.02479	34.24	34.48	-0.24
17.00	15.05	0.02789	0.03013	34.28	34.38	-0.10
17.50	0.0	0.19754	0.02852	32.03	33.53	-1.51
17.50	2.93	0.12769	0.02827	32.88	34.14	-1.26
17.50	5.85	0.11564	0.02601	33.74	34.33	-0.60
17.50	8.78	0.02376	0.02796	34.16	34.41	-0.25
17.50	11.71	-0.04500	0.02630	34.32	34.53	-0.21
17.50	14.63	0.02652	0.03176	34.35	34.38	-0.04
18.00	0.0	0.02417	0.02093	32.33	33.60	-1.26
18.00	2.84	0.01244	0.02467	33.10	34.15	-1.05
18.00	5.69	0.06220	0.01980	33.89	34.27	-0.39
18.00	8.53	-0.02043	0.02220	34.24	34.35	-0.11
18.00	11.37	-0.07277	0.02317	34.35	34.48	-0.13
18.00	14.22	0.01469	0.02269	34.37	34.35	0.02
18.50	0.0	-0.14134	0.01178	33.55	33.55	0.0
18.50	2.76	-0.10639	0.02170	34.06	34.06	0.0
18.50	5.52	-0.00933	0.01684	34.13	34.13	0.0
18.50	8.28	-0.06779	0.01114	34.20	34.20	0.0
18.50	11.04	-0.10993	0.02299	34.33	34.33	0.0
18.50	13.80	0.00002	0.0	34.26	34.26	0.0

STEP= 13 TIME=13:00 hr

X (km)	Y (m)	U (m/s)	Variance (m/s)	Simulated (ppm)	Kriged (ppm)	Difference (ppm)
0.0	0.0	0.95052	0.00521	0.0	0.0	0.0
0.0	0.46	0.90969	0.00308	0.08	0.08	0.0
0.0	0.92	0.93500	0.00146	0.09	0.09	0.0
0.0	1.38	0.75689	0.00186	0.09	0.09	0.0
0.0	1.84	0.39997	0.00399	0.70	0.70	0.0
0.0	2.30	0.0	0.0	1.55	1.55	0.0
0.50	0.0	0.92943	0.01021	0.17	0.29	-0.12
0.50	0.44	0.87017	0.00822	0.17	0.84	-0.67
0.50	0.88	0.81142	0.00797	0.17	1.09	-0.91
0.50	1.31	0.66821	0.00785	0.29	1.32	-1.03
0.50	1.75	0.42252	0.00816	0.54	1.79	-1.25
0.50	2.19	0.15309	0.00836	0.58	2.51	-1.93
1.00	0.0	0.88312	0.01606	0.31	0.96	-0.66
1.00	0.41	0.79984	0.01426	0.30	1.48	-1.17
1.00	0.83	0.70416	0.01373	0.33	1.89	-1.56
1.00	1.24	0.57310	0.01366	0.43	2.30	-1.87
1.00	1.66	0.40113	0.01384	0.59	2.81	-2.22
1.00	2.07	0.21350	0.01436	0.69	3.47	-2.78
1.50	0.0	0.82191	0.01974	0.49	1.65	-1.16
1.50	0.39	0.72743	0.01812	0.51	2.13	-1.62
1.50	0.78	0.62310	0.01746	0.58	2.60	-2.02
1.50	1.18	0.50292	0.01735	0.72	3.10	-2.38
1.50	1.57	0.36696	0.01760	0.90	3.66	-2.76
1.50	1.96	0.22435	0.01823	0.99	4.32	-3.33
2.00	0.0	0.75965	0.02093	0.67	2.35	-1.68
2.00	0.37	0.66290	0.01941	0.71	2.78	-2.07
2.00	0.74	0.55925	0.01871	0.84	3.25	-2.41
2.00	1.11	0.44766	0.01859	1.06	3.77	-2.72
2.00	1.48	0.33025	0.01893	1.31	4.37	-3.06
2.00	1.85	0.21223	0.01969	1.43	5.05	-3.62
2.50	0.0	0.70271	0.01961	1.00	3.06	-2.06
2.50	0.35	0.60891	0.01809	1.09	3.43	-2.34
2.50	0.69	0.50904	0.01738	1.31	3.85	-2.54
2.50	1.04	0.40284	0.01727	1.64	4.36	-2.72
2.50	1.39	0.29381	0.01768	1.97	4.97	-3.01
2.50	1.74	0.18812	0.01860	2.09	5.68	-3.59
3.00	0.0	0.65359	0.01588	1.38	3.83	-2.45
3.00	0.32	0.56778	0.01429	1.48	4.09	-2.61
3.00	0.65	0.47525	0.01361	1.76	4.43	-2.66
3.00	0.97	0.37151	0.01348	2.19	4.89	-2.70
3.00	1.30	0.26033	0.01386	2.65	5.50	-2.85
3.00	1.62	0.15531	0.01492	2.88	6.24	-3.36
3.50	0.0	0.60959	0.01009	2.07	4.71	-2.64
3.50	0.30	0.53848	0.00828	2.24	4.84	-2.60
3.50	0.60	0.46751	0.00798	2.70	5.03	-2.33
3.50	0.91	0.37396	0.00773	3.32	5.37	-2.05
3.50	1.21	0.23973	0.00775	3.78	5.97	-2.19
3.50	1.51	0.10908	0.00871	3.84	6.77	-2.94
4.00	0.0	0.56522	0.00497	2.79	5.88	-3.09
4.00	0.28	0.49691	0.00059	2.89	5.91	-3.02
4.00	0.56	0.46765	0.00371	3.15	6.01	-2.86
4.00	0.84	0.43756	0.00257	3.60	6.08	-2.47
4.00	1.12	0.29414	0.00171	4.38	6.53	-2.15
4.00	1.40	0.0	0.0	5.24	7.52	-2.28
4.50	0.0	0.54147	0.00968	3.77	7.53	-3.76
4.50	0.44	0.44615	0.00781	4.33	7.77	-3.44
4.50	0.88	0.33238	0.00753	6.07	8.22	-2.15
4.50	1.32	0.14727	0.00765	8.92	9.17	-0.24
4.50	1.76	0.00697	0.01004	12.15	10.46	1.70
4.50	2.20	-0.06331	0.01428	14.69	11.80	2.89
5.00	0.0	0.51635	0.01443	5.07	9.46	-4.39

5.00	0.60	0.37307	0.01248	6.58	10.08	-3.50
5.00	1.20	0.20500	0.01241	10.60	11.12	-0.51
5.00	1.80	0.04856	0.01398	15.79	12.59	3.20
5.00	2.39	-0.05309	0.01706	20.30	14.23	6.08
5.00	2.99	-0.12038	0.02029	23.06	15.85	7.21
5.50	0.0	0.49429	0.01646	6.59	11.47	-4.88
5.50	0.76	0.32086	0.01444	9.19	12.52	-3.32
5.50	1.52	0.14222	0.01472	15.13	14.02	1.10
5.50	2.27	-0.00088	0.01636	21.18	15.86	5.32
5.50	3.03	-0.09462	0.01850	25.55	17.75	7.80
5.50	3.79	-0.16037	0.02037	27.70	19.54	8.15
6.00	0.0	0.47675	0.01556	8.18	13.47	-5.29
6.00	0.92	0.29010	0.01344	11.76	14.92	-3.16
6.00	1.83	0.10098	0.01382	18.84	16.84	2.00
6.00	2.75	-0.03492	0.01482	24.90	18.93	5.98
6.00	3.67	-0.12420	0.01586	28.53	20.96	7.57
6.00	4.59	-0.19145	0.01671	30.07	22.83	7.24
6.50	0.0	0.45965	0.01182	9.77	15.41	-5.65
6.50	1.08	0.27759	0.00977	14.15	17.22	-3.07
6.50	2.15	0.06151	0.01004	21.87	19.54	2.33
6.50	3.23	-0.05443	0.01042	27.40	21.70	5.70
6.50	4.31	-0.15973	0.01076	30.25	23.84	6.41
6.50	5.38	-0.19538	0.01107	31.27	25.67	5.60
7.00	0.0	0.43722	0.00610	11.32	17.26	-5.94
7.00	1.24	0.27907	0.00476	16.28	19.36	-3.08
7.00	2.47	0.03179	0.00573	24.20	21.94	2.26
7.00	3.71	-0.07238	0.00514	29.07	24.19	4.89
7.00	4.94	-0.22795	0.00374	31.20	26.33	4.88
7.00	6.18	-0.08479	0.00382	31.86	27.95	3.91
7.50	0.0	0.43398	0.00685	12.85	18.91	-6.06
7.50	1.34	0.25648	0.00594	17.87	21.19	-3.32
7.50	2.68	0.03158	0.00588	25.41	23.71	1.70
7.50	4.02	-0.10410	0.00493	29.78	25.97	3.81
7.50	5.36	-0.21069	0.00602	31.57	27.95	3.62
7.50	6.70	-0.03866	0.00607	32.05	29.18	2.88
8.00	0.0	0.44095	0.01070	14.31	20.39	-6.07
8.00	1.41	0.23704	0.00918	19.10	22.67	-3.57
8.00	2.81	0.02522	0.00915	26.04	25.11	0.94
8.00	4.22	-0.14016	0.00918	30.09	27.17	2.92
8.00	5.63	-0.19910	0.00923	31.73	29.01	2.73
8.00	7.03	-0.07580	0.01098	32.16	30.06	2.09
8.50	0.0	0.44038	0.01070	15.68	21.76	-6.08
8.50	1.47	0.23031	0.00918	20.16	23.92	-3.76
8.50	2.95	0.00957	0.00911	26.65	26.36	0.29
8.50	4.42	-0.16718	0.00921	30.37	28.10	2.27
8.50	5.89	-0.21977	0.00912	31.87	29.91	1.96
8.50	7.37	-0.07748	0.01028	32.24	30.79	1.45
9.00	0.0	0.43698	0.00683	16.97	23.04	-6.07
9.00	1.54	0.23177	0.00617	21.18	24.98	-3.80
9.00	3.08	-0.01637	0.00500	27.20	27.57	-0.37
9.00	4.62	-0.19817	0.00605	30.65	28.77	1.89
9.00	6.16	-0.24622	0.00526	31.99	30.78	1.21
9.00	7.70	-0.03974	0.00555	32.28	31.31	0.98
9.50	0.0	0.42578	0.00583	18.22	24.26	-6.04
9.50	1.56	0.23507	0.00555	21.99	25.93	-3.94
9.50	3.11	-0.00983	0.00385	27.45	28.34	-0.89
9.50	4.67	-0.19380	0.00519	30.73	29.28	1.45
9.50	6.22	-0.24168	0.00457	32.01	31.24	0.77
9.50	7.78	-0.02135	0.00395	32.29	31.61	0.67
10.00	0.0	0.40412	0.00996	19.47	25.44	-5.97
10.00	1.50	0.23545	0.00856	22.59	26.83	-4.25
10.00	2.99	0.04814	0.00840	27.33	28.52	-1.19
10.00	4.49	-0.12811	0.00856	30.51	29.73	0.79
10.00	5.98	-0.20538	0.00839	31.91	31.23	0.67
10.00	7.48	-0.05569	0.00926	32.24	31.76	0.48
10.50	0.0	0.38140	0.01040	20.69	26.56	-5.87

10.50	1.44	0.23855	0.00893	23.22	27.62	-4.40
10.50	2.87	0.09800	0.00886	27.30	28.73	-1.43
10.50	4.31	-0.06812	0.00891	30.31	30.01	0.30
10.50	5.74	-0.15601	0.00887	31.79	31.27	0.52
10.50	7.18	-0.05777	0.01029	32.19	31.79	0.39
11.00	0.0	0.35826	0.00678	21.85	27.59	-5.74
11.00	1.38	0.24302	0.00600	23.86	28.25	-4.38
11.00	2.75	0.14322	0.00557	27.33	28.92	-1.59
11.00	4.13	-0.01226	0.00511	30.14	30.12	0.02
11.00	5.50	-0.11124	0.00616	31.69	31.33	0.36
11.00	6.88	-0.03018	0.00582	32.17	31.76	0.41
11.50	0.0	0.34968	0.00594	22.88	28.23	-5.35
11.50	1.43	0.24583	0.00558	24.72	28.68	-3.96
11.50	2.85	0.15714	0.00412	27.97	29.20	-1.24
11.50	4.28	0.00598	0.00498	30.57	30.39	0.18
11.50	5.71	-0.08350	0.00505	31.92	31.48	0.44
11.50	7.13	-0.01834	0.00795	32.39	31.66	0.73
12.00	0.0	0.36055	0.01078	23.74	28.38	-4.65
12.00	1.64	0.24415	0.00926	25.82	28.93	-3.12
12.00	3.29	0.12863	0.00930	29.26	29.63	-0.37
12.00	4.93	-0.01946	0.00922	31.52	30.86	0.65
12.00	6.57	-0.04521	0.00926	32.45	31.47	0.97
12.00	8.22	-0.05228	0.01663	32.82	31.52	1.30
12.50	0.0	0.37062	0.01268	24.50	28.48	-3.97
12.50	1.86	0.24072	0.01116	26.84	29.09	-2.25
12.50	3.72	0.10728	0.01126	30.31	29.94	0.37
12.50	5.58	-0.04456	0.01133	32.14	31.02	1.13
12.50	7.44	-0.06745	0.01308	32.81	31.32	1.49
12.50	9.30	-0.06135	0.01675	33.10	31.51	1.59
13.00	0.0	0.37688	0.01083	25.21	28.58	-3.37
13.00	2.08	0.23669	0.00951	27.77	29.24	-1.47
13.00	4.15	0.09035	0.00962	31.13	30.16	0.98
13.00	6.23	-0.07617	0.00978	32.57	31.04	1.53
13.00	8.31	-0.08884	0.01113	33.07	31.22	1.85
13.00	10.38	-0.04521	0.01213	33.34	31.82	1.51
13.50	0.0	0.37792	0.00595	25.87	28.75	-2.88
13.50	2.29	0.23206	0.00589	28.61	29.49	-0.88
13.50	4.59	0.06673	0.00857	31.78	30.48	1.30
13.50	6.88	-0.09389	0.00997	32.87	31.19	1.68
13.50	9.17	-0.07298	0.01013	33.29	31.39	1.90
13.50	11.47	-0.01561	0.00751	33.54	32.76	0.78
14.00	0.0	0.36695	0.00699	26.51	29.29	-2.78
14.00	2.44	0.22860	0.00795	29.29	30.04	-0.74
14.00	4.88	0.05072	0.01021	32.19	30.97	1.22
14.00	7.32	-0.09255	0.00952	33.07	31.48	1.59
14.00	9.76	-0.05365	0.00634	33.46	31.69	1.77
14.00	12.20	-0.01300	0.00728	33.71	33.42	0.29
14.50	0.0	0.34532	0.01154	27.16	30.13	-2.97
14.50	2.54	0.22452	0.01125	29.86	30.77	-0.90
14.50	5.08	0.05083	0.01185	32.47	31.58	0.90
14.50	7.62	-0.07251	0.01087	33.22	32.00	1.23
14.50	10.16	-0.04199	0.01047	33.61	32.41	1.20
14.50	12.70	-0.03104	0.01384	33.86	33.82	0.05
15.00	0.0	0.31764	0.01269	27.80	31.01	-3.21
15.00	2.64	0.21774	0.01217	30.38	31.55	-1.17
15.00	5.28	0.05748	0.01226	32.72	32.27	0.45
15.00	7.92	-0.04524	0.01152	33.38	32.65	0.73
15.00	10.56	-0.03872	0.01207	33.76	33.12	0.64
15.00	13.20	-0.04349	0.01470	34.01	34.10	-0.09
15.50	0.0	0.28405	0.01006	28.44	31.88	-3.44
15.50	2.74	0.20659	0.01093	30.84	32.29	-1.45
15.50	5.48	0.06496	0.01022	32.94	32.96	-0.02
15.50	8.22	-0.02131	0.00914	33.54	33.32	0.22
15.50	10.96	-0.04729	0.01127	33.92	33.68	0.24
15.50	13.70	-0.04823	0.01037	34.12	34.25	-0.13
16.00	0.0	0.24657	0.00517	29.07	32.66	-3.59

16.00	2.84	0.18554	0.00974	31.26	32.91	-1.64
16.00	5.68	0.06845	0.00562	33.13	33.57	-0.44
16.00	8.52	-0.00948	0.00780	33.71	33.85	-0.14
16.00	11.36	-0.06540	0.00877	34.07	34.05	0.02
16.00	14.20	-0.02226	0.00206	34.18	34.29	-0.11
16.50	0.0	0.21906	0.00810	29.71	33.03	-3.32
16.50	2.79	0.15169	0.01035	31.56	33.29	-1.74
16.50	5.59	0.06906	0.00845	33.22	33.86	-0.64
16.50	8.38	-0.00078	0.00824	33.84	34.18	-0.34
16.50	11.17	-0.08181	0.01045	34.16	34.26	-0.10
16.50	13.97	-0.02554	0.00672	34.21	34.24	-0.03
17.00	0.0	0.19344	0.01213	30.38	33.19	-2.81
17.00	2.71	0.10368	0.01199	31.88	33.49	-1.61
17.00	5.42	0.05687	0.01174	33.33	33.98	-0.65
17.00	8.13	0.00315	0.01100	33.96	34.31	-0.35
17.00	10.84	-0.09922	0.01215	34.22	34.40	-0.18
17.00	13.55	-0.01799	0.01292	34.26	34.23	0.02
17.50	0.0	0.16495	0.01253	31.25	33.30	-2.05
17.50	2.63	0.04771	0.01212	32.41	33.58	-1.17
17.50	5.25	0.03273	0.01224	33.53	34.02	-0.48
17.50	7.88	0.00423	0.01139	34.06	34.33	-0.27
17.50	10.51	-0.11210	0.01193	34.24	34.47	-0.22
17.50	13.13	-0.01493	0.01404	34.28	34.25	0.03
18.00	0.0	0.13505	0.00920	32.33	33.38	-1.06
18.00	2.54	-0.01116	0.00982	33.13	33.60	-0.47
18.00	5.09	-0.00061	0.01090	33.79	34.01	-0.22
18.00	7.63	0.00112	0.00896	34.14	34.30	-0.16
18.00	10.17	-0.11182	0.00813	34.27	34.46	-0.19
18.00	12.72	-0.01703	0.00997	34.26	34.27	-0.01
18.50	0.0	0.10182	0.00519	33.48	33.48	0.0
18.50	2.46	-0.06536	0.00717	33.62	33.62	0.0
18.50	4.92	-0.03980	0.01003	33.99	33.99	0.0
18.50	7.38	-0.01481	0.00865	34.24	34.24	0.0
18.50	9.84	-0.10217	0.00299	34.39	34.39	0.0
18.50	12.30	0.0	-0.0	34.29	34.29	0.0

STEPE= 17 TIME=15:00 hr

X (km)	Y (m)	U (m/s)	Variance (m/s)	Simulated (ppm)	Kriged (ppm)	Difference (ppm)
0.0	0.0	-0.50298	0.00190	0.23	0.23	0.0
0.0	0.82	-0.48592	0.00030	0.90	0.90	0.0
0.0	1.64	-0.46143	0.00093	0.91	0.91	0.0
0.0	2.46	-0.38573	0.00115	0.92	0.92	0.0
0.0	3.28	-0.21988	0.00094	1.58	1.58	0.0
0.0	4.10	-0.00054	-0.0	3.45	3.45	0.0
0.50	0.0	-0.50789	0.02150	1.94	1.51	0.43
0.50	0.79	-0.48362	0.02064	1.60	2.40	-0.80
0.50	1.58	-0.45212	0.02015	1.31	2.67	-1.37
0.50	2.37	-0.33877	0.02024	0.94	2.93	-1.99
0.50	3.16	-0.17233	0.02121	0.72	3.61	-2.90
0.50	3.95	0.07735	0.02282	0.72	5.17	-4.45
1.00	0.0	-0.53518	0.05871	2.12	2.59	-0.46
1.00	0.76	-0.52079	0.05685	2.21	3.66	-1.45
1.00	1.52	-0.47214	0.05561	1.96	4.34	-2.38
1.00	2.28	-0.33658	0.05572	1.40	4.96	-3.56
1.00	3.04	-0.11545	0.05825	0.90	5.81	-4.91
1.00	3.80	0.14438	0.06310	0.71	7.08	-6.37
1.50	0.0	-0.56798	0.08626	3.47	3.64	-0.18
1.50	0.73	-0.57784	0.08286	3.46	4.84	-1.39
1.50	1.46	-0.50326	0.08155	3.17	5.88	-2.72
1.50	2.19	-0.34995	0.08157	2.33	6.87	-4.54
1.50	2.92	-0.09086	0.08473	1.42	7.90	-6.48
1.50	3.65	0.21174	0.09256	1.02	9.06	-8.04
2.00	0.0	-0.59136	0.09164	4.51	4.66	-0.16
2.00	0.70	-0.60950	0.08696	4.75	5.96	-1.22
2.00	1.40	-0.55911	0.08581	4.79	7.31	-2.53
2.00	2.10	-0.38323	0.08572	3.83	8.65	-4.82
2.00	2.80	-0.09678	0.08845	2.41	9.88	-7.47
2.00	3.50	0.25422	0.09777	1.69	11.04	-9.35
2.50	0.0	-0.60362	0.07460	5.93	5.63	0.31
2.50	0.67	-0.65814	0.06953	6.33	6.98	-0.65
2.50	1.34	-0.63001	0.06874	6.84	8.62	-1.78
2.50	2.01	-0.46484	0.06856	6.12	10.33	-4.21
2.50	2.68	-0.13119	0.07012	4.16	11.79	-7.63
2.50	3.35	0.25722	0.07854	2.95	12.98	-10.03
3.00	0.0	-0.61799	0.04410	7.25	6.52	0.73
3.00	0.64	-0.67800	0.03985	7.81	7.84	-0.03
3.00	1.28	-0.69234	0.03959	8.91	9.76	-0.85
3.00	1.92	-0.57400	0.03942	9.02	11.96	-2.93
3.00	2.56	-0.21094	0.03978	7.01	13.66	-6.65
3.00	3.20	0.22133	0.04499	5.24	14.87	-9.63
3.50	0.0	-0.57523	0.01459	8.64	7.38	1.26
3.50	0.61	-0.64938	0.01206	9.27	8.51	0.76
3.50	1.22	-0.71740	0.01213	10.74	10.62	0.12
3.50	1.83	-0.68937	0.01204	11.90	13.60	-1.70
3.50	2.44	-0.34512	0.01214	10.96	15.57	-4.61
3.50	3.05	0.14388	0.01331	9.02	16.70	-7.68
4.00	0.0	-0.51552	0.00170	9.97	8.40	1.56
4.00	0.58	-0.61431	0.00064	10.60	9.32	1.28
4.00	1.16	-0.69830	0.00028	12.15	11.18	0.97
4.00	1.74	-0.76322	0.00063	13.97	15.07	-1.10
4.00	2.32	-0.50198	0.00082	14.57	17.37	-2.80
4.00	2.90	-0.00074	-0.0	14.08	18.36	-4.28
4.50	0.0	-0.43898	0.01187	11.08	9.85	1.24
4.50	0.74	-0.58238	0.01026	12.14	11.48	0.66
4.50	1.48	-0.72437	0.01042	14.59	14.82	-0.24
4.50	2.22	-0.58343	0.01031	16.92	18.27	-1.34
4.50	2.96	-0.06800	0.01017	17.00	20.05	-3.05
4.50	3.70	0.32637	0.02446	16.91	21.31	-4.40
5.00	0.0	-0.31586	0.02955	12.01	11.42	0.59

5.00	0.90	-0.56063	0.02686	13.64	13.91	-0.27
5.00	1.80	-0.66425	0.02682	17.07	17.71	-0.64
5.00	2.70	-0.34803	0.02675	20.17	20.83	-0.67
5.00	3.59	0.07461	0.03344	21.01	22.76	-1.75
5.00	4.49	0.30287	0.06504	21.59	24.03	-2.44
5.50	0.0	-0.19570	0.03852	12.84	12.90	-0.07
5.50	1.06	-0.50928	0.03493	15.10	16.08	-0.98
5.50	2.12	-0.58041	0.03486	19.46	20.27	-0.82
5.50	3.17	-0.28860	0.03551	23.38	23.44	-0.06
5.50	4.23	-0.01509	0.04869	25.71	25.29	0.42
5.50	5.29	0.12369	0.07652	27.13	26.33	0.81
6.00	0.0	-0.06627	0.03267	13.56	14.23	-0.67
6.00	1.22	-0.47778	0.02897	16.59	18.05	-1.47
6.00	2.43	-0.56505	0.02889	21.75	22.81	-1.06
6.00	3.65	-0.37648	0.03058	26.01	25.92	0.09
6.00	4.87	-0.18975	0.04072	28.85	27.42	1.43
6.00	6.09	-0.07659	0.05430	30.20	28.12	2.08
6.50	0.0	0.01955	0.01676	14.35	15.40	-1.05
6.50	1.38	-0.47960	0.01409	18.16	19.98	-1.82
6.50	2.75	-0.61763	0.01399	23.76	25.31	-1.55
6.50	4.13	-0.51823	0.01503	27.79	28.06	-0.26
6.50	5.51	-0.37427	0.01867	30.20	29.04	1.16
6.50	6.88	-0.18912	0.02194	31.14	29.42	1.72
7.00	0.0	0.06211	0.00321	15.25	16.53	-1.28
7.00	1.54	-0.51256	0.00230	19.70	22.03	-2.33
7.00	3.07	-0.69173	0.00148	25.33	27.56	-2.23
7.00	4.61	-0.61676	0.00234	28.97	29.52	-0.55
7.00	6.14	-0.53623	0.00192	30.93	30.24	0.69
7.00	7.68	-0.07987	0.00262	31.62	29.99	1.63
7.50	0.0	0.01453	0.00404	16.41	18.30	-1.89
7.50	1.64	-0.55654	0.00318	20.85	23.86	-3.00
7.50	3.28	-0.74812	0.00305	26.18	28.71	-2.53
7.50	4.92	-0.67719	0.00281	29.51	30.19	-0.68
7.50	6.56	-0.61704	0.00365	31.24	30.77	0.47
7.50	8.20	-0.03746	0.00373	31.81	30.20	1.60
8.00	0.0	-0.08359	0.01152	17.69	20.55	-2.86
8.00	1.71	-0.56692	0.00997	21.72	25.31	-3.58
8.00	3.41	-0.74747	0.01005	26.72	29.14	-2.42
8.00	5.12	-0.70393	0.01033	29.84	30.38	-0.54
8.00	6.83	-0.61275	0.01094	31.42	30.84	0.57
8.00	8.53	-0.12597	0.01365	31.92	30.39	1.53
8.50	0.0	-0.20750	0.01125	18.85	22.73	-3.88
8.50	1.77	-0.56238	0.00958	22.50	26.59	-4.09
8.50	3.55	-0.69736	0.00969	27.22	29.35	-2.13
8.50	5.32	-0.69434	0.00991	30.13	30.37	-0.24
8.50	7.09	-0.55423	0.01024	31.55	30.79	0.76
8.50	8.87	-0.20917	0.01277	31.99	30.55	1.44
9.00	0.0	-0.29699	0.00387	19.84	24.71	-4.87
9.00	1.84	-0.52871	0.00250	23.24	27.63	-4.39
9.00	3.68	-0.62043	0.00285	27.71	29.50	-1.79
9.00	5.52	-0.66164	0.00309	30.45	30.37	0.08
9.00	7.36	-0.47748	0.00302	31.69	30.79	0.90
9.00	9.20	-0.16311	0.00307	32.01	30.76	1.25
9.50	0.0	-0.30852	0.00262	20.69	26.17	-5.48
9.50	1.85	-0.48707	0.00130	23.85	28.36	-4.52
9.50	3.71	-0.56436	0.00170	28.04	29.78	-1.74
9.50	5.56	-0.62122	0.00199	30.63	30.54	0.08
9.50	7.42	-0.43132	0.00198	31.76	30.96	0.80
9.50	9.27	-0.12366	0.00149	32.00	31.10	0.90
10.00	0.0	-0.22554	0.00961	21.46	27.03	-5.57
10.00	1.79	-0.44725	0.00810	24.30	28.84	-4.54
10.00	3.58	-0.55439	0.00821	28.14	30.26	-2.12
10.00	5.37	-0.58846	0.00824	30.64	30.93	-0.29
10.00	7.16	-0.44012	0.00822	31.77	31.30	0.47
10.00	8.94	-0.20617	0.01041	31.97	31.46	0.51
10.50	0.0	-0.09865	0.01099	22.17	27.74	-5.57

10.50	1.72	-0.38307	0.00958	24.73	29.11	-4.39
10.50	3.45	-0.55007	0.00964	28.28	30.81	-2.53
10.50	5.17	-0.56688	0.00957	30.67	31.49	-0.82
10.50	6.90	-0.46659	0.00962	31.81	31.70	0.11
10.50	8.62	-0.10707	0.01223	31.99	31.87	0.12
11.00	0.0	0.03927	0.00405	22.84	28.41	-5.57
11.00	1.66	-0.30192	0.00324	25.17	29.27	-4.10
11.00	3.32	-0.55006	0.00321	28.47	31.33	-2.86
11.00	4.98	-0.55985	0.00272	30.74	32.08	-1.33
11.00	6.64	-0.49525	0.00333	31.88	32.14	-0.26
11.00	8.29	-0.01262	0.00339	32.09	32.26	-0.17
11.50	0.0	0.14632	0.00366	23.48	28.97	-5.49
11.50	1.70	-0.24739	0.00218	25.82	29.67	-3.85
11.50	3.41	-0.53767	0.00244	29.03	31.92	-2.89
11.50	5.11	-0.55645	0.00172	31.16	32.57	-1.42
11.50	6.82	-0.43263	0.00189	32.10	32.56	-0.47
11.50	8.52	0.16848	0.00743	32.31	32.70	-0.40
12.00	0.0	0.20905	0.02228	24.10	29.39	-5.29
12.00	1.92	-0.26027	0.01775	26.79	30.51	-3.72
12.00	3.83	-0.51919	0.01775	30.06	32.58	-2.52
12.00	5.75	-0.51238	0.01782	31.89	32.94	-1.05
12.00	7.67	-0.09354	0.01812	32.45	32.98	-0.54
12.00	9.59	0.49993	0.08547	32.50	33.22	-0.72
12.50	0.0	0.23199	0.05270	24.71	29.83	-5.12
12.50	2.13	-0.29378	0.04471	27.73	31.30	-3.58
12.50	4.26	-0.51237	0.04459	30.91	33.00	-2.09
12.50	6.39	-0.40744	0.04465	32.38	33.26	-0.88
12.50	8.52	0.19668	0.05445	32.66	33.37	-0.71
12.50	10.65	0.69644	0.19466	32.64	33.65	-1.02
13.00	0.0	0.22623	0.08255	25.31	30.28	-4.97
13.00	2.34	-0.33135	0.07189	28.62	31.95	-3.34
13.00	4.68	-0.49117	0.07165	31.61	33.33	-1.72
13.00	7.03	-0.24435	0.07187	32.76	33.54	-0.78
13.00	9.37	0.33524	0.11242	32.84	33.71	-0.87
13.00	11.71	0.75691	0.27276	32.78	33.97	-1.19
13.50	0.0	0.19518	0.10063	25.93	30.71	-4.78
13.50	2.55	-0.36283	0.08891	29.46	32.48	-3.02
13.50	5.11	-0.44828	0.08861	32.21	33.59	-1.38
13.50	7.66	-0.10163	0.08998	33.06	33.77	-0.71
13.50	10.22	0.36316	0.15409	33.03	33.98	-0.95
13.50	12.77	0.75478	0.29518	32.94	34.15	-1.21
14.00	0.0	0.14663	0.10033	26.62	31.11	-4.49
14.00	2.65	-0.37638	0.08935	30.11	32.84	-2.74
14.00	5.30	-0.40783	0.08900	32.57	33.76	-1.20
14.00	7.96	-0.08995	0.09104	33.32	33.94	-0.62
14.00	10.61	0.26525	0.14139	33.27	34.14	-0.87
14.00	13.26	0.63637	0.23765	33.09	34.22	-1.14
14.50	0.0	0.09032	0.08151	27.37	31.48	-4.11
14.50	2.67	-0.38207	0.07294	30.63	33.11	-2.47
14.50	5.35	-0.37595	0.07260	32.82	33.88	-1.06
14.50	8.02	-0.14237	0.07344	33.56	34.04	-0.48
14.50	10.69	0.12647	0.10110	33.57	34.23	-0.66
14.50	13.37	0.42774	0.14900	33.26	34.27	-1.00
15.00	0.0	0.02907	0.05086	28.15	31.82	-3.67
15.00	2.69	-0.38578	0.04618	31.13	33.32	-2.19
15.00	5.39	-0.34793	0.04571	33.06	33.95	-0.90
15.00	8.08	-0.19915	0.04470	33.76	34.09	-0.34
15.00	10.78	-0.00308	0.05790	33.83	34.27	-0.43
15.00	13.47	0.24401	0.07407	33.46	34.27	-0.81
15.50	0.0	-0.02805	0.02032	28.95	32.11	-3.17
15.50	2.71	-0.38391	0.02060	31.61	33.50	-1.89
15.50	5.43	-0.32714	0.01942	33.28	33.99	-0.72
15.50	8.14	-0.25544	0.01630	33.90	34.10	-0.20
15.50	10.86	-0.11336	0.02409	34.01	34.27	-0.27
15.50	13.57	0.09791	0.02255	33.61	34.24	-0.64
16.00	0.0	-0.07848	0.00378	29.76	32.37	-2.62

16.00	2.74	-0.37038	0.00811	32.08	33.63	-1.55
16.00	5.47	-0.31256	0.00568	33.47	34.00	-0.54
16.00	8.21	-0.30011	0.00158	33.97	34.08	-0.10
16.00	10.94	-0.19965	0.00937	34.10	34.26	-0.16
16.00	13.68	0.00812	0.00062	33.67	34.19	-0.52
16.50	0.0	-0.11707	0.00864	30.60	32.63	-2.04
16.50	2.73	-0.34281	0.01199	32.50	33.70	-1.20
16.50	5.46	-0.30829	0.01011	33.59	33.98	-0.40
16.50	8.19	-0.32992	0.00675	33.96	34.06	-0.10
16.50	10.92	-0.26196	0.01328	34.13	34.23	-0.09
16.50	13.65	-0.06750	0.00735	33.78	34.13	-0.35
17.00	0.0	-0.14395	0.02112	31.49	32.87	-1.38
17.00	2.72	-0.30367	0.02201	32.91	33.73	-0.81
17.00	5.43	-0.30637	0.02099	33.66	33.93	-0.27
17.00	8.15	-0.34160	0.01896	33.90	34.03	-0.13
17.00	10.87	-0.29132	0.02334	34.09	34.18	-0.09
17.00	13.59	-0.09691	0.02163	33.91	34.06	-0.15
17.50	0.0	-0.15997	0.02358	32.38	33.08	-0.70
17.50	2.70	-0.25864	0.02409	33.25	33.71	-0.46
17.50	5.41	-0.30642	0.02336	33.67	33.85	-0.19
17.50	8.11	-0.33789	0.02130	33.80	33.95	-0.15
17.50	10.82	-0.28161	0.02502	33.99	34.10	-0.11
17.50	13.52	-0.10013	0.02391	34.00	33.97	0.03
18.00	0.0	-0.16409	0.01226	33.06	33.25	-0.19
18.00	2.69	-0.21274	0.01488	33.47	33.66	-0.19
18.00	5.38	-0.30282	0.01422	33.64	33.75	-0.11
18.00	8.08	-0.32128	0.01012	33.72	33.84	-0.12
18.00	10.77	-0.24785	0.01519	33.84	33.96	-0.12
18.00	13.46	-0.06907	0.01124	33.94	33.84	0.10
18.50	0.0	-0.15367	0.00364	33.35	33.35	0.0
18.50	2.68	-0.17304	0.00718	33.58	33.58	0.0
18.50	5.36	-0.29165	0.00670	33.63	33.63	0.0
18.50	8.04	-0.29845	0.00005	33.69	33.69	0.0
18.50	10.72	-0.20944	0.00694	33.77	33.77	0.0
18.50	13.40	0.00102	-0.0	33.64	33.64	0.0

STEP= 23 TIME=18:00 hr

X (km)	Y (m)	U (m/s)	Variance (m/s)	Simulated (ppm)	Kriged (ppm)	Difference (ppm)
0.0	0.0	-0.54600	0.02007	21.83	21.83	0.0
0.0	1.68	-0.73720	0.01356	22.94	22.94	0.0
0.0	3.36	-0.78311	0.01358	23.82	23.82	0.0
0.0	5.04	-0.68767	0.01350	24.44	24.44	0.0
0.0	6.72	-0.45823	0.01384	24.79	24.79	0.0
0.0	8.40	-0.11717	0.01872	24.87	24.87	0.0
0.50	0.0	-0.56608	0.01850	16.37	22.51	-6.13
0.50	1.62	-0.74238	0.01376	17.48	23.63	-6.15
0.50	3.24	-0.77950	0.01379	20.27	24.55	-4.28
0.50	4.87	-0.68712	0.01379	20.45	25.22	-4.77
0.50	6.49	-0.47581	0.01439	16.22	25.63	-9.41
0.50	8.11	-0.16931	0.01680	14.19	25.78	-11.58
1.00	0.0	-0.58169	0.01869	20.74	23.15	-2.42
1.00	1.56	-0.74267	0.01471	22.14	24.28	-2.15
1.00	3.13	-0.77545	0.01461	23.71	25.23	-1.53
1.00	4.69	-0.68145	0.01469	25.22	25.95	-0.73
1.00	6.26	-0.48694	0.01577	24.58	26.41	-1.82
1.00	7.82	-0.21439	0.01796	20.16	26.61	-6.46
1.50	0.0	-0.58874	0.01921	19.02	23.77	-4.74
1.50	1.51	-0.74077	0.01544	19.84	24.90	-5.06
1.50	3.01	-0.76784	0.01520	22.13	25.86	-3.74
1.50	4.52	-0.67702	0.01530	23.25	26.61	-3.36
1.50	6.03	-0.49421	0.01673	22.47	27.12	-4.65
1.50	7.54	-0.25239	0.01945	21.87	27.38	-5.51
2.00	0.0	-0.58859	0.01940	21.10	24.35	-3.25
2.00	1.45	-0.73096	0.01560	22.27	25.47	-3.20
2.00	2.90	-0.75587	0.01524	23.98	26.45	-2.47
2.00	4.35	-0.66874	0.01532	25.88	27.22	-1.35
2.00	5.80	-0.50054	0.01682	26.01	27.77	-1.76
2.00	7.25	-0.28509	0.02002	24.06	28.08	-4.02
2.50	0.0	-0.58277	0.01909	20.71	24.91	-4.19
2.50	1.39	-0.71441	0.01524	21.42	26.01	-4.58
2.50	2.78	-0.73968	0.01482	23.27	26.98	-3.71
2.50	4.18	-0.66098	0.01485	24.86	27.77	-2.92
2.50	5.57	-0.50604	0.01618	25.67	28.35	-2.68
2.50	6.96	-0.31390	0.01944	25.59	28.70	-3.11
3.00	0.0	-0.56793	0.01842	21.76	25.44	-3.68
3.00	1.34	-0.69211	0.01459	22.67	26.51	-3.84
3.00	2.67	-0.71918	0.01418	24.25	27.47	-3.22
3.00	4.01	-0.65081	0.01415	26.11	28.27	-2.16
3.00	5.34	-0.51034	0.01516	27.12	28.87	-1.74
3.00	6.68	-0.34017	0.01805	26.76	29.25	-2.49
3.50	0.0	-0.54689	0.01765	21.93	25.94	-4.01
3.50	1.28	-0.66097	0.01395	22.57	26.98	-4.41
3.50	2.56	-0.69166	0.01359	24.05	27.92	-3.86
3.50	3.83	-0.63599	0.01352	25.60	28.71	-3.11
3.50	5.11	-0.51472	0.01418	27.10	29.32	-2.21
3.50	6.39	-0.36609	0.01640	27.69	29.73	-2.04
4.00	0.0	-0.51954	0.01700	22.52	26.43	-3.91
4.00	1.22	-0.62567	0.01350	23.22	27.42	-4.20
4.00	2.44	-0.65920	0.01321	24.59	28.32	-3.74
4.00	3.66	-0.61788	0.01314	26.14	29.10	-2.95
4.00	4.88	-0.51710	0.01348	27.55	29.71	-2.16
4.00	6.10	-0.39029	0.01496	28.35	30.14	-1.79
4.50	0.0	-0.48759	0.01656	22.89	26.89	-4.00
4.50	1.40	-0.59572	0.01319	23.66	28.01	-4.36
4.50	2.81	-0.61519	0.01305	25.24	29.01	-3.77
4.50	4.21	-0.54954	0.01304	26.87	29.83	-2.95
4.50	5.62	-0.43047	0.01376	28.41	30.42	-2.01
4.50	7.02	-0.31030	0.01612	29.41	30.77	-1.36
5.00	0.0	-0.45208	0.01631	23.25	27.33	-4.08

5.00	1.59	-0.56077	0.01312	24.24	28.58	-4.33
5.00	3.18	-0.56779	0.01306	26.08	29.65	-3.56
5.00	4.77	-0.48629	0.01311	27.93	30.47	-2.53
5.00	6.35	-0.37264	0.01422	29.47	30.99	-1.53
5.00	7.94	-0.27054	0.01695	30.32	31.24	-0.92
5.50	0.0	-0.41633	0.01614	23.67	27.75	-4.08
5.50	1.77	-0.52377	0.01313	24.80	29.10	-4.29
5.50	3.55	-0.52123	0.01309	26.84	30.21	-3.37
5.50	5.32	-0.43807	0.01320	28.75	31.00	-2.25
5.50	7.09	-0.34754	0.01449	30.22	31.45	-1.23
5.50	8.87	-0.25173	0.01686	30.96	31.58	-0.62
6.00	0.0	-0.38318	0.01597	24.01	28.15	-4.15
6.00	1.96	-0.48621	0.01311	25.32	29.58	-4.25
6.00	3.91	-0.47954	0.01303	27.56	30.70	-3.14
6.00	5.87	-0.41160	0.01319	29.57	31.44	-1.87
6.00	7.83	-0.34658	0.01435	30.90	31.78	-0.89
6.00	9.79	-0.22850	0.01599	31.43	31.81	-0.37
6.50	0.0	-0.35464	0.01575	24.42	28.53	-4.11
6.50	2.14	-0.45220	0.01299	25.90	30.01	-4.11
6.50	4.28	-0.44699	0.01289	28.32	31.12	-2.80
6.50	6.43	-0.40636	0.01304	30.32	31.78	-1.46
6.50	8.57	-0.35242	0.01385	31.40	32.02	-0.63
6.50	10.71	-0.18117	0.01506	31.71	31.95	-0.24
7.00	0.0	-0.33193	0.01551	24.77	28.88	-4.12
7.00	2.33	-0.42293	0.01283	26.42	30.40	-3.98
7.00	4.65	-0.42634	0.01270	29.02	31.46	-2.44
7.00	6.98	-0.41465	0.01281	30.95	32.03	-1.09
7.00	9.30	-0.34737	0.01327	31.76	32.18	-0.42
7.00	11.63	-0.10497	0.01520	31.85	32.03	-0.19
7.50	0.0	-0.31785	0.01528	25.18	29.22	-4.03
7.50	2.41	-0.39920	0.01266	26.90	30.68	-3.79
7.50	4.81	-0.41472	0.01255	29.53	31.68	-2.14
7.50	7.22	-0.42773	0.01258	31.34	32.18	-0.84
7.50	9.62	-0.35244	0.01279	31.97	32.30	-0.33
7.50	12.03	-0.08515	0.01507	31.92	32.15	-0.23
8.00	0.0	-0.30980	0.01510	25.58	29.53	-3.95
8.00	2.42	-0.38048	0.01254	27.26	30.90	-3.64
8.00	4.83	-0.40585	0.01244	29.85	31.81	-1.96
8.00	7.25	-0.43643	0.01244	31.58	32.27	-0.69
8.00	9.66	-0.36573	0.01255	32.13	32.39	-0.26
8.00	12.08	-0.10533	0.01417	32.02	32.28	-0.26
8.50	0.0	-0.30794	0.01496	26.00	29.83	-3.83
8.50	2.42	-0.36784	0.01246	27.65	31.10	-3.45
8.50	4.85	-0.39820	0.01237	30.17	31.92	-1.75
8.50	7.27	-0.43877	0.01237	31.81	32.33	-0.52
8.50	9.70	-0.36813	0.01245	32.28	32.45	-0.17
8.50	12.12	-0.11648	0.01373	32.12	32.39	-0.27
9.00	0.0	-0.31016	0.01487	26.40	30.11	-3.70
9.00	2.43	-0.35954	0.01242	27.99	31.28	-3.28
9.00	4.87	-0.39122	0.01233	30.44	32.01	-1.57
9.00	7.30	-0.43497	0.01234	32.01	32.38	-0.37
9.00	9.74	-0.36057	0.01241	32.43	32.50	-0.07
9.00	12.17	-0.11948	0.01356	32.22	32.48	-0.27
9.50	0.0	-0.31277	0.01482	26.79	30.37	-3.57
9.50	2.43	-0.35351	0.01241	28.31	31.44	-3.12
9.50	4.85	-0.38345	0.01231	30.65	32.09	-1.44
9.50	7.28	-0.42551	0.01232	32.17	32.41	-0.24
9.50	9.70	-0.34940	0.01238	32.59	32.55	0.04
9.50	12.13	-0.12525	0.01338	32.36	32.57	-0.21
10.00	0.0	-0.31241	0.01483	27.15	30.62	-3.47
10.00	2.39	-0.34677	0.01242	28.57	31.58	-3.02
10.00	4.78	-0.37332	0.01232	30.78	32.15	-1.37
10.00	7.17	-0.41145	0.01233	32.28	32.44	-0.16
10.00	9.56	-0.33832	0.01237	32.75	32.58	0.16
10.00	11.95	-0.13692	0.01313	32.56	32.65	-0.09
10.50	0.0	-0.30707	0.01488	27.48	30.86	-3.39

10.50	2.36	-0.33666	0.01246	28.82	31.72	-2.90
10.50	4.71	-0.36054	0.01236	30.92	32.22	-1.30
10.50	7.07	-0.39372	0.01236	32.39	32.48	-0.08
10.50	9.42	-0.32204	0.01237	32.90	32.62	0.27
10.50	11.78	-0.14082	0.01301	32.79	32.72	0.07
11.00	0.0	-0.29419	0.01497	27.77	31.10	-3.33
11.00	2.32	-0.32075	0.01254	29.06	31.87	-2.80
11.00	4.64	-0.34361	0.01243	31.06	32.30	-1.24
11.00	6.96	-0.37253	0.01242	32.50	32.52	-0.02
11.00	9.28	-0.30243	0.01242	33.03	32.67	0.37
11.00	11.60	-0.13903	0.01294	33.01	32.78	0.23
11.50	0.0	-0.27259	0.01511	28.05	31.33	-3.28
11.50	2.39	-0.29757	0.01267	29.40	32.03	-2.64
11.50	4.78	-0.32482	0.01256	31.38	32.41	-1.03
11.50	7.17	-0.34530	0.01255	32.75	32.60	0.15
11.50	9.56	-0.25757	0.01253	33.20	32.74	0.45
11.50	11.95	-0.09868	0.01340	33.19	32.88	0.31
12.00	0.0	-0.24321	0.01530	28.32	31.56	-3.24
12.00	2.61	-0.26761	0.01285	29.86	32.23	-2.38
12.00	5.23	-0.30542	0.01272	31.91	32.55	-0.64
12.00	7.84	-0.30208	0.01271	33.13	32.72	0.41
12.00	10.46	-0.17482	0.01274	33.38	32.87	0.50
12.00	13.07	-0.02785	0.01508	33.28	33.04	0.24
12.50	0.0	-0.20766	0.01550	28.62	31.79	-3.17
12.50	2.84	-0.23238	0.01303	30.33	32.42	-2.09
12.50	5.68	-0.27946	0.01291	32.38	32.69	-0.31
12.50	8.52	-0.24686	0.01290	33.40	32.85	0.55
12.50	11.36	-0.10066	0.01318	33.50	33.02	0.47
12.50	14.20	0.00887	0.01660	33.32	33.20	0.12
13.00	0.0	-0.16930	0.01569	28.97	32.02	-3.05
13.00	3.06	-0.19442	0.01321	30.81	32.61	-1.80
13.00	6.13	-0.24705	0.01310	32.77	32.84	-0.06
13.00	9.19	-0.18673	0.01309	33.60	32.99	0.61
13.00	12.26	-0.04614	0.01375	33.60	33.18	0.41
13.00	15.32	0.01883	0.01729	33.36	33.36	-0.00
13.50	0.0	-0.13096	0.01588	29.38	32.25	-2.87
13.50	3.29	-0.15634	0.01335	31.29	32.79	-1.50
13.50	6.58	-0.20963	0.01326	33.10	32.98	0.12
13.50	9.87	-0.12917	0.01325	33.73	33.14	0.59
13.50	13.16	-0.01397	0.01421	33.68	33.35	0.33
13.50	16.45	0.01173	0.01772	33.39	33.51	-0.12
14.00	0.0	-0.09743	0.01608	29.90	32.48	-2.59
14.00	3.44	-0.11938	0.01348	31.73	32.97	-1.25
14.00	6.88	-0.17055	0.01340	33.31	33.13	0.18
14.00	10.33	-0.08869	0.01340	33.80	33.28	0.52
14.00	13.77	-0.00435	0.01427	33.78	33.50	0.29
14.00	17.21	-0.00016	0.01784	33.47	33.64	-0.17
14.50	0.0	-0.07206	0.01627	30.51	32.71	-2.21
14.50	3.55	-0.08663	0.01358	32.14	33.15	-1.01
14.50	7.09	-0.13461	0.01351	33.46	33.28	0.18
14.50	10.64	-0.06245	0.01352	33.84	33.43	0.42
14.50	14.19	-0.00521	0.01420	33.87	33.62	0.25
14.50	17.73	-0.00950	0.01739	33.59	33.75	-0.16
15.00	0.0	-0.05594	0.01647	31.22	32.95	-1.73
15.00	3.65	-0.06189	0.01368	32.56	33.34	-0.78
15.00	7.30	-0.10539	0.01361	33.59	33.44	0.15
15.00	10.95	-0.04652	0.01362	33.87	33.57	0.30
15.00	14.60	-0.01110	0.01421	33.92	33.75	0.17
15.00	18.25	-0.01296	0.01685	33.71	33.86	-0.15
15.50	0.0	-0.05288	0.01666	32.00	33.19	-1.19
15.50	3.75	-0.04770	0.01377	32.97	33.53	-0.55
15.50	7.51	-0.08684	0.01369	33.70	33.60	0.10
15.50	11.26	-0.04321	0.01371	33.87	33.71	0.16
15.50	15.02	-0.02139	0.01433	33.93	33.86	0.07
15.50	18.77	-0.01369	0.01660	33.79	33.95	-0.16
16.00	0.0	-0.06384	0.01682	32.77	33.42	-0.66

16.00	3.86	-0.04766	0.01387	33.35	33.72	-0.37
16.00	7.72	-0.08255	0.01377	33.78	33.76	0.03
16.00	11.58	-0.05285	0.01380	33.87	33.84	0.03
16.00	15.44	-0.03547	0.01450	33.91	33.97	-0.06
16.00	19.30	-0.00647	0.01870	33.84	34.03	-0.19
16.50	0.0	-0.08965	0.01694	33.37	33.66	-0.29
16.50	3.78	-0.06117	0.01398	33.63	33.90	-0.27
16.50	7.57	-0.09442	0.01383	33.83	33.91	-0.08
16.50	11.35	-0.08003	0.01386	33.87	33.96	-0.09
16.50	15.13	-0.05620	0.01441	33.87	34.04	-0.17
16.50	18.92	-0.01616	0.01687	33.87	34.10	-0.23
17.00	0.0	-0.13174	0.01708	33.71	33.89	-0.18
17.00	3.66	-0.09360	0.01407	33.82	34.09	-0.27
17.00	7.32	-0.12325	0.01385	33.89	34.08	-0.19
17.00	10.99	-0.12175	0.01386	33.90	34.08	-0.18
17.00	14.65	-0.09039	0.01423	33.85	34.12	-0.26
17.00	18.31	-0.03102	0.01643	33.83	34.16	-0.33
17.50	0.0	-0.19074	0.01745	33.91	34.12	-0.21
17.50	3.54	-0.14581	0.01412	33.99	34.28	-0.30
17.50	7.08	-0.17058	0.01385	34.00	34.24	-0.24
17.50	10.62	-0.17660	0.01384	33.98	34.20	-0.22
17.50	14.17	-0.13988	0.01407	33.92	34.19	-0.28
17.50	17.71	-0.05554	0.01640	33.79	34.22	-0.43
18.00	0.0	-0.26912	0.01859	34.22	34.35	-0.13
18.00	3.42	-0.21844	0.01432	34.30	34.48	-0.18
18.00	6.84	-0.23826	0.01400	34.26	34.41	-0.15
18.00	10.26	-0.24783	0.01399	34.19	34.33	-0.14
18.00	13.68	-0.20501	0.01411	34.12	34.28	-0.16
18.00	17.10	-0.09915	0.01599	33.95	34.26	-0.32
18.50	0.0	-0.36516	0.02158	34.58	34.58	0.0
18.50	3.30	-0.31128	0.01514	34.67	34.67	0.0
18.50	6.60	-0.32640	0.01477	34.57	34.57	0.0
18.50	9.90	-0.33591	0.01477	34.46	34.46	0.0
18.50	13.20	-0.28706	0.01482	34.37	34.37	0.0
18.50	16.50	-0.16034	0.01598	34.32	34.32	0.0